



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:01 AM UTC

PDB ID : 3BS0 / pdb_00003bs0
Title : Crystal structure of the P. putida toluene transporter TodX
Authors : Hearn, E.M.; Patel, D.R.; van den Berg, B.
Deposited on : 2007-12-21
Resolution : 2.60 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

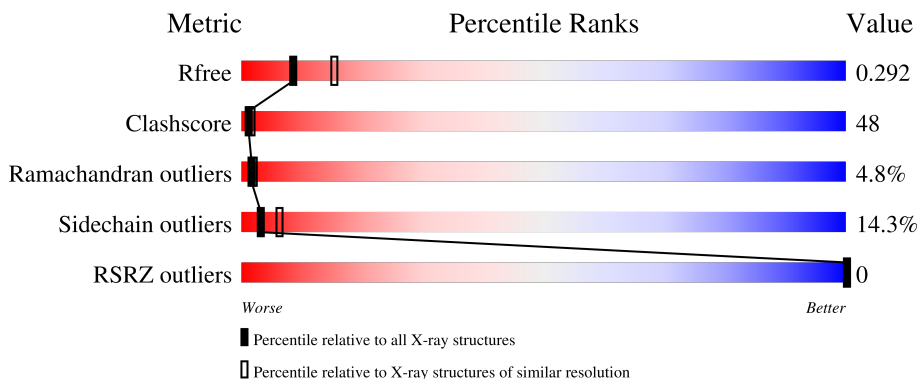
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	439	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 6%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>40% 40% 13% • 6%</div>
1	B	439	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 39%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 6%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>40% 39% 13% • 6%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6410 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.

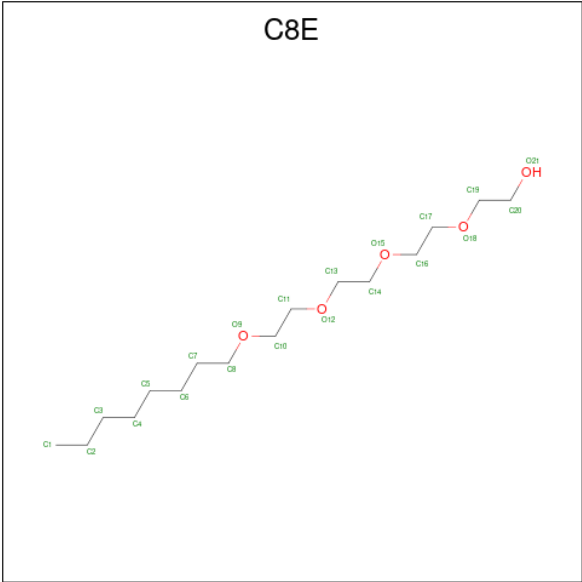
- Molecule 1 is a protein called TodX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3119	1974	533	606	6			
1	B	414	Total	C	N	O	S	0	0	0
			3119	1974	533	606	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	PRO	variant	UNP Q51971
A	77	GLY	ALA	variant	UNP Q51971
A	434	HIS	-	expression tag	UNP Q51971
A	435	HIS	-	expression tag	UNP Q51971
A	436	HIS	-	expression tag	UNP Q51971
A	437	HIS	-	expression tag	UNP Q51971
A	438	HIS	-	expression tag	UNP Q51971
A	439	HIS	-	expression tag	UNP Q51971
B	434	HIS	-	expression tag	UNP Q51971
B	435	HIS	-	expression tag	UNP Q51971
B	436	HIS	-	expression tag	UNP Q51971
B	437	HIS	-	expression tag	UNP Q51971
B	438	HIS	-	expression tag	UNP Q51971
B	439	HIS	-	expression tag	UNP Q51971

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	6	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	6	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		

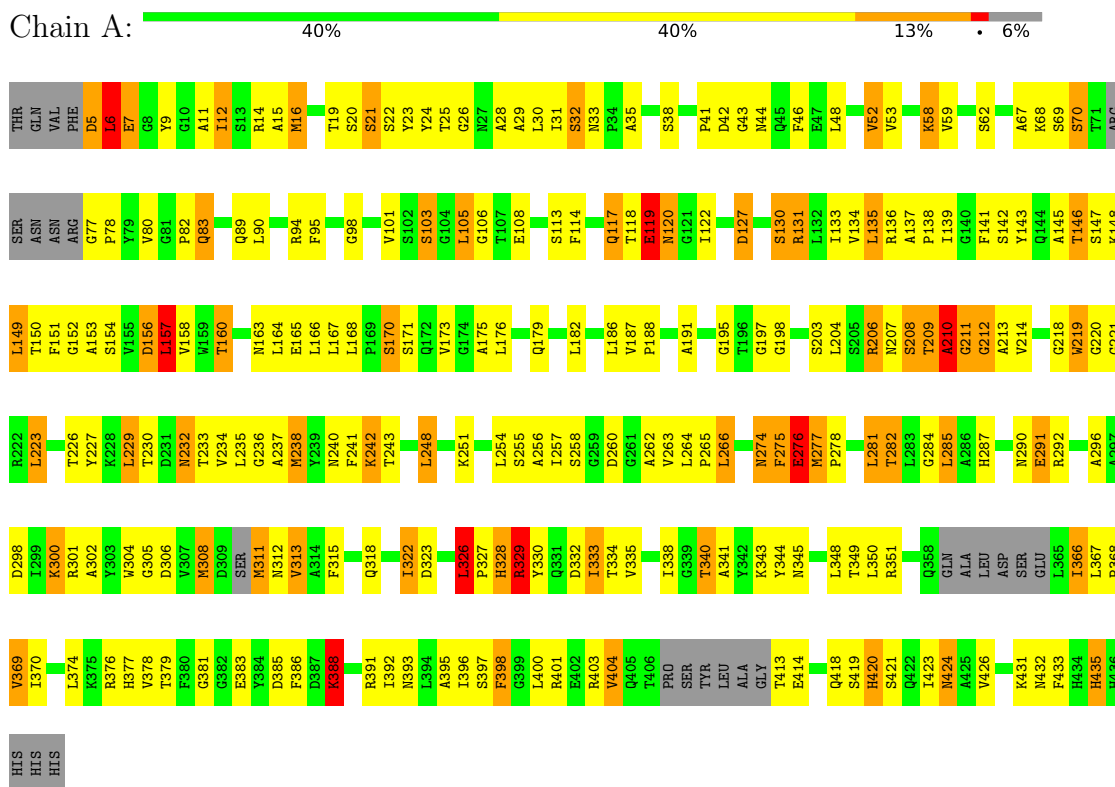
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	47	Total	O	0	0
			47	47		

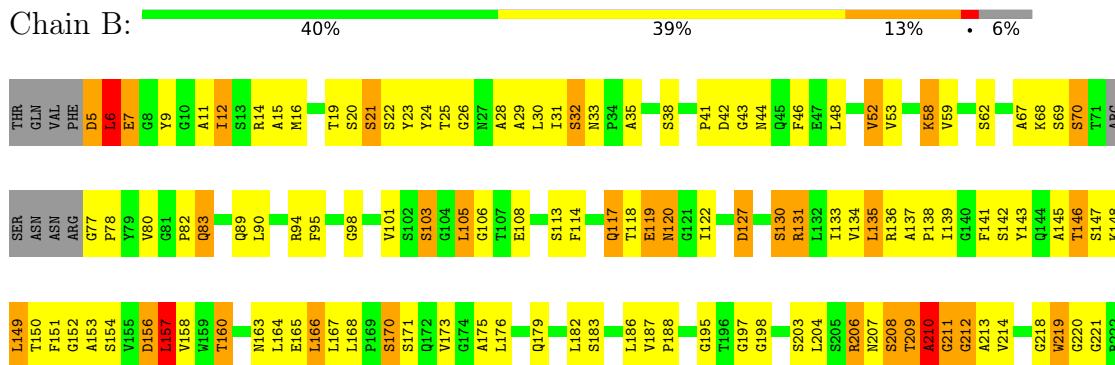
3 Residue-property plots

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: TodX



• Molecule 1: TodX





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.10Å 41.41Å 141.06Å 98.39° 90.01° 90.06°	Depositor
Resolution (Å)	11.98 – 2.60 11.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.1 (11.98-2.60) 90.9 (11.98-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.291 0.251 , 0.292	Depositor DCC
R_{free} test set	1189 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l 0.051 for -h,k,-k-l 0.048 for -h,-k,k+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6410	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: C8E

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	0.57	1/3182 (0.0%)	1.19	37/4316 (0.9%)
1	B	0.57	0/3182	1.19	37/4316 (0.9%)
All	All	0.57	1/6364 (0.0%)	1.19	74/8632 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	MET	SD-CE	-5.03	1.67	1.79

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ALA	N-CA-C	-12.28	84.64	110.80
1	B	210	ALA	N-CA-C	-12.28	84.65	110.80
1	B	156	ASP	N-CA-C	11.20	125.92	108.12
1	A	156	ASP	N-CA-C	11.16	125.86	108.12
1	A	77	GLY	CA-C-N	9.88	131.17	120.11
1	A	77	GLY	C-N-CA	9.88	131.17	120.11
1	B	77	GLY	CA-C-N	9.81	131.10	120.11
1	B	77	GLY	C-N-CA	9.81	131.10	120.11
1	A	209	THR	N-CA-C	9.00	126.47	107.67
1	B	209	THR	N-CA-C	9.00	126.47	107.67
1	B	212	GLY	N-CA-C	-8.89	92.10	113.18
1	A	212	GLY	N-CA-C	-8.87	92.17	113.18
1	B	78	PRO	N-CA-C	8.34	123.25	111.33
1	A	78	PRO	N-CA-C	8.32	123.23	111.33
1	A	208	SER	N-CA-C	8.30	122.11	108.08
1	B	208	SER	N-CA-C	8.29	122.09	108.08
1	B	264	LEU	CA-C-N	7.83	127.78	120.03
1	B	264	LEU	C-N-CA	7.83	127.78	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	LEU	CA-C-N	7.83	127.78	120.03
1	A	264	LEU	C-N-CA	7.83	127.78	120.03
1	A	119	GLU	N-CA-C	-7.02	95.85	110.80
1	B	119	GLU	N-CA-C	-6.97	95.96	110.80
1	A	31	ILE	CB-CA-C	-6.86	104.71	111.30
1	B	31	ILE	CB-CA-C	-6.79	104.78	111.30
1	A	308	MET	N-CA-C	-6.47	105.92	113.88
1	B	308	MET	N-CA-C	-6.43	105.98	113.88
1	A	139	ILE	N-CA-C	-6.40	99.15	108.11
1	B	139	ILE	N-CA-C	-6.39	99.17	108.11
1	B	166	LEU	N-CA-C	6.22	118.82	108.13
1	A	388	LYS	N-CA-C	-6.20	105.58	113.02
1	A	166	LEU	N-CA-C	6.18	118.77	108.13
1	B	388	LYS	N-CA-C	-6.16	105.63	113.02
1	B	165	GLU	N-CA-C	-6.13	96.95	107.61
1	A	165	GLU	N-CA-C	-6.09	97.00	107.61
1	B	103	SER	N-CA-C	-6.07	101.48	110.46
1	A	103	SER	N-CA-C	-6.05	101.50	110.46
1	A	248	LEU	N-CA-C	-6.04	100.16	109.76
1	B	248	LEU	N-CA-C	-6.01	100.21	109.76
1	A	206	ARG	N-CA-C	5.99	119.15	110.28
1	B	206	ARG	N-CA-C	5.98	119.13	110.28
1	A	326	LEU	CA-C-N	5.97	129.24	120.46
1	A	326	LEU	C-N-CA	5.97	129.24	120.46
1	B	326	LEU	CA-C-N	5.97	129.23	120.46
1	B	326	LEU	C-N-CA	5.97	129.23	120.46
1	A	274	ASN	N-CA-C	5.95	123.48	110.80
1	A	62	SER	N-CA-C	-5.94	105.89	113.02
1	B	274	ASN	N-CA-C	5.94	123.45	110.80
1	B	62	SER	N-CA-C	-5.92	105.91	113.02
1	A	53	VAL	N-CA-C	5.89	114.83	106.53
1	B	53	VAL	N-CA-C	5.89	114.83	106.53
1	A	275	PHE	N-CA-C	-5.80	99.70	108.46
1	B	275	PHE	N-CA-C	-5.78	99.73	108.46
1	B	276	GLU	N-CA-C	-5.62	98.84	110.80
1	B	170	SER	N-CA-C	5.61	118.12	111.33
1	A	276	GLU	N-CA-C	-5.60	98.88	110.80
1	A	277	MET	N-CA-C	-5.59	97.47	109.81
1	B	277	MET	N-CA-C	-5.56	97.52	109.81
1	A	170	SER	N-CA-C	5.53	118.02	111.33
1	A	195	GLY	N-CA-C	5.53	121.12	111.50
1	B	195	GLY	N-CA-C	5.50	121.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	SER	N-CA-C	5.42	117.94	111.71
1	B	21	SER	N-CA-C	5.40	117.92	111.71
1	B	420	HIS	N-CA-C	5.40	117.23	108.26
1	B	206	ARG	CA-C-N	-5.39	114.35	122.81
1	B	206	ARG	C-N-CA	-5.39	114.35	122.81
1	A	206	ARG	CA-C-N	-5.38	114.36	122.81
1	A	206	ARG	C-N-CA	-5.38	114.36	122.81
1	B	330	TYR	N-CA-C	5.37	118.97	109.96
1	A	420	HIS	N-CA-C	5.36	117.16	108.26
1	A	330	TYR	N-CA-C	5.30	118.87	109.96
1	A	327	PRO	N-CA-C	5.19	118.72	110.21
1	B	327	PRO	N-CA-C	5.16	118.68	110.21
1	B	329	ARG	N-CA-C	-5.12	99.89	110.80
1	A	329	ARG	N-CA-C	-5.12	99.89	110.80

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	3119	0	3039	296	0
1	B	3119	0	3039	305	0
2	A	42	0	68	1	0
2	B	42	0	68	7	0
3	A	41	0	0	3	0
3	B	47	0	0	8	0
All	All	6410	0	6214	599	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 48.

All (599) 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:5:ASP:OD1	1:A:300:LYS:HE2	1.58	1.04
1:B:5:ASP:OD1	1:B:300:LYS:HE2	1.58	1.04
1:A:311:MET:HE3	1:A:326:LEU:O	1.61	1.01
1:B:311:MET:HE3	1:B:326:LEU:O	1.61	1.01
1:A:15:ALA:HB1	1:A:381:GLY:HA3	1.43	1.00
1:B:15:ALA:HB1	1:B:381:GLY:HA3	1.43	1.00
1:B:238:MET:HG3	3:B:544:HOH:O	1.66	0.93
1:A:275:PHE:CZ	1:A:311:MET:SD	2.63	0.91
1:A:311:MET:HE2	1:A:328:HIS:CE1	2.05	0.91
1:B:275:PHE:CZ	1:B:311:MET:SD	2.63	0.91
1:B:311:MET:HE2	1:B:328:HIS:CE1	2.05	0.91
1:A:401:ARG:HB2	1:A:421:SER:HB3	1.50	0.91
1:B:145:ALA:HB3	1:B:149:LEU:HD11	1.52	0.90
1:B:401:ARG:HB2	1:B:421:SER:HB3	1.51	0.90
1:A:145:ALA:HB3	1:A:149:LEU:HD11	1.52	0.90
1:B:366:ILE:HG23	1:B:367:LEU:H	1.37	0.90
1:A:366:ILE:HG23	1:A:367:LEU:H	1.37	0.89
1:A:243:THR:CG2	1:A:277:MET:HB2	2.04	0.88
1:A:230:THR:HG23	1:A:232:ASN:H	1.38	0.88
1:B:230:THR:HG23	1:B:232:ASN:H	1.38	0.88
1:B:243:THR:CG2	1:B:277:MET:HB2	2.04	0.88
1:B:134:VAL:HG22	1:B:160:THR:HG23	1.58	0.86
1:A:134:VAL:HG22	1:A:160:THR:HG23	1.58	0.86
1:B:311:MET:SD	1:B:326:LEU:CD1	2.65	0.85
1:A:119:GLU:O	1:A:120:ASN:HB2	1.74	0.85
1:B:119:GLU:O	1:B:120:ASN:HB2	1.74	0.85
1:A:311:MET:SD	1:A:326:LEU:CD1	2.65	0.85
1:A:369:VAL:HG12	1:A:370:ILE:HD12	1.58	0.84
1:B:118:THR:CG2	1:B:198:GLY:HA2	2.08	0.84
1:A:5:ASP:CG	1:A:6:LEU:N	2.36	0.84
1:B:369:VAL:HG12	1:B:370:ILE:HD12	1.58	0.84
1:B:5:ASP:CG	1:B:6:LEU:N	2.36	0.84
1:B:229:LEU:H	1:B:229:LEU:HD23	1.42	0.84
1:A:118:THR:CG2	1:A:198:GLY:HA2	2.08	0.83
1:A:229:LEU:HD23	1:A:229:LEU:H	1.43	0.83
1:B:16:MET:O	1:B:19:THR:HG22	1.77	0.83
1:A:16:MET:O	1:A:19:THR:HG22	1.77	0.83
1:A:207:ASN:OD1	1:A:208:SER:N	2.12	0.82
1:B:207:ASN:OD1	1:B:208:SER:N	2.12	0.82
1:A:175:ALA:O	1:A:179:GLN:HG3	1.81	0.81
1:B:175:ALA:O	1:B:179:GLN:HG3	1.80	0.81
1:B:118:THR:HG21	1:B:198:GLY:HA2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:A:198:GLY:HA2	1.62	0.80
1:A:376:ARG:HB2	1:A:400:LEU:HD12	1.64	0.79
1:B:376:ARG:HB2	1:B:400:LEU:HD12	1.65	0.79
1:B:326:LEU:O	1:B:326:LEU:HD12	1.83	0.78
1:A:41:PRO:HG2	1:A:432:ASN:HD21	1.48	0.78
1:A:326:LEU:O	1:A:326:LEU:HD12	1.83	0.78
1:B:41:PRO:HG2	1:B:432:ASN:HD21	1.48	0.78
1:B:214:VAL:HG12	1:B:248:LEU:HB3	1.65	0.78
1:A:214:VAL:HG12	1:A:248:LEU:HB3	1.65	0.78
1:A:230:THR:HG22	1:A:233:THR:HB	1.65	0.78
1:B:230:THR:HG22	1:B:233:THR:HB	1.65	0.77
1:B:145:ALA:HB3	1:B:149:LEU:CD1	2.13	0.77
1:A:145:ALA:HB3	1:A:149:LEU:CD1	2.13	0.77
1:A:275:PHE:HZ	1:A:311:MET:SD	2.05	0.77
1:A:403:ARG:NH1	3:A:528:HOH:O	2.15	0.77
1:B:275:PHE:HZ	1:B:311:MET:SD	2.05	0.77
1:B:52:VAL:HG13	1:B:80:VAL:HG22	1.67	0.75
1:A:52:VAL:HG13	1:A:80:VAL:HG22	1.67	0.75
1:A:276:GLU:O	1:A:277:MET:HG3	1.87	0.75
1:B:276:GLU:O	1:B:277:MET:HG3	1.87	0.75
1:A:16:MET:HE2	1:A:341:ALA:HB2	1.69	0.74
1:A:401:ARG:NH1	1:A:419:SER:HB2	2.02	0.74
1:B:243:THR:HG21	1:B:277:MET:HB2	1.68	0.74
1:B:401:ARG:NH1	1:B:419:SER:HB2	2.02	0.74
1:A:376:ARG:CB	1:A:400:LEU:HD12	2.18	0.74
1:B:16:MET:HE2	1:B:341:ALA:HB2	1.69	0.74
1:B:376:ARG:CB	1:B:400:LEU:HD12	2.18	0.74
1:A:243:THR:HG21	1:A:277:MET:HB2	1.68	0.74
1:B:156:ASP:O	1:B:157:LEU:HB3	1.87	0.74
1:A:156:ASP:O	1:A:157:LEU:HB3	1.87	0.74
1:A:351:ARG:HH12	1:A:383:GLU:HB2	1.54	0.73
1:B:351:ARG:HH12	1:B:383:GLU:HB2	1.53	0.73
1:B:15:ALA:CB	1:B:381:GLY:HA3	2.18	0.73
1:A:15:ALA:CB	1:A:381:GLY:HA3	2.18	0.73
1:A:131:ARG:HG2	1:A:131:ARG:HH11	1.55	0.72
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.55	0.71
1:A:38:SER:HB2	1:A:150:THR:HG21	1.73	0.71
1:B:38:SER:HB2	1:B:150:THR:HG21	1.73	0.71
1:B:395:ALA:C	1:B:396:ILE:HD12	2.14	0.71
1:A:210:ALA:O	1:A:212:GLY:N	2.24	0.71
1:B:210:ALA:O	1:B:212:GLY:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ALA:C	1:A:396:ILE:HD12	2.15	0.70
1:B:313:VAL:HG11	2:B:504:C8E:H112	1.73	0.70
1:B:313:VAL:CG1	2:B:504:C8E:H112	2.22	0.70
1:A:15:ALA:HB1	1:A:381:GLY:CA	2.19	0.70
1:B:15:ALA:HB1	1:B:381:GLY:CA	2.19	0.70
1:A:119:GLU:O	1:A:120:ASN:CB	2.41	0.69
1:B:119:GLU:O	1:B:120:ASN:CB	2.41	0.69
1:B:203:SER:C	1:B:204:LEU:HD12	2.17	0.69
1:A:203:SER:C	1:A:204:LEU:HD12	2.18	0.69
1:A:233:THR:OG1	1:A:287:HIS:HD2	1.76	0.68
1:B:233:THR:OG1	1:B:287:HIS:HD2	1.76	0.68
1:B:16:MET:HE3	1:B:351:ARG:CD	2.23	0.68
1:A:16:MET:HE3	1:A:351:ARG:CD	2.23	0.68
1:A:143:TYR:CE2	1:A:145:ALA:HA	2.29	0.67
1:B:143:TYR:CE2	1:B:145:ALA:HA	2.29	0.67
1:B:43:GLY:HA2	1:B:435:HIS:CE1	2.30	0.67
1:A:302:ALA:HB3	1:A:333:ILE:CG2	2.24	0.67
1:A:43:GLY:HA2	1:A:435:HIS:CE1	2.30	0.67
1:B:368:PRO:HA	1:B:418:GLN:HE22	1.59	0.67
1:A:46:PHE:CD2	1:A:431:LYS:HE3	2.29	0.67
1:B:302:ALA:HB3	1:B:333:ILE:CG2	2.24	0.67
1:B:46:PHE:CD2	1:B:431:LYS:HE3	2.29	0.67
1:B:212:GLY:O	1:B:213:ALA:HB3	1.95	0.67
1:A:212:GLY:O	1:A:213:ALA:HB3	1.95	0.66
1:A:368:PRO:HA	1:A:418:GLN:HE22	1.60	0.66
1:A:59:VAL:HG21	1:A:368:PRO:HB3	1.77	0.66
1:A:366:ILE:HG23	1:A:367:LEU:N	2.10	0.66
1:B:59:VAL:HG21	1:B:368:PRO:HB3	1.77	0.66
1:B:366:ILE:HG23	1:B:367:LEU:N	2.10	0.66
1:A:311:MET:SD	1:A:326:LEU:HD12	2.35	0.65
1:B:311:MET:SD	1:B:326:LEU:HD12	2.35	0.65
1:A:14:ARG:HH11	1:A:424:ASN:HD22	1.43	0.65
1:B:379:THR:HG22	1:B:397:SER:CB	2.27	0.65
1:A:401:ARG:HH11	1:A:419:SER:HB2	1.62	0.65
1:B:14:ARG:HH11	1:B:424:ASN:HD22	1.44	0.65
1:A:328:HIS:O	1:A:329:ARG:HB2	1.96	0.65
1:A:379:THR:HG22	1:A:397:SER:CB	2.27	0.65
1:B:229:LEU:H	1:B:229:LEU:CD2	2.09	0.65
1:B:328:HIS:O	1:B:329:ARG:HB2	1.96	0.65
1:B:206:ARG:HG2	1:B:211:GLY:O	1.97	0.65
1:A:131:ARG:HG2	1:A:131:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:HB	1:A:226:THR:OG1	1.98	0.64
1:A:157:LEU:HD12	1:A:157:LEU:C	2.20	0.64
1:B:157:LEU:C	1:B:157:LEU:HD12	2.20	0.64
1:B:401:ARG:HH11	1:B:419:SER:HB2	1.62	0.64
1:A:229:LEU:H	1:A:229:LEU:CD2	2.09	0.64
1:A:206:ARG:HG2	1:A:211:GLY:O	1.98	0.64
1:B:150:THR:HB	1:B:226:THR:OG1	1.98	0.64
1:B:151:PHE:HD2	1:B:152:GLY:H	1.44	0.64
1:A:151:PHE:HD2	1:A:152:GLY:H	1.44	0.64
1:A:254:LEU:HD22	1:A:322:ILE:CD1	2.27	0.64
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.11	0.64
1:A:333:ILE:HG12	1:A:334:THR:N	2.12	0.64
1:B:333:ILE:HG12	1:B:334:THR:N	2.13	0.63
1:B:254:LEU:HD22	1:B:322:ILE:CD1	2.27	0.63
1:B:149:LEU:HA	1:B:226:THR:O	1.98	0.63
1:A:149:LEU:HA	1:A:226:THR:O	1.98	0.63
1:B:186:LEU:HB2	1:B:322:ILE:HG23	1.81	0.62
1:B:12:ILE:HD12	1:B:351:ARG:NE	2.13	0.62
1:A:12:ILE:HD12	1:A:351:ARG:NE	2.13	0.62
1:A:186:LEU:HB2	1:A:322:ILE:HG23	1.82	0.62
1:B:5:ASP:CG	1:B:6:LEU:H	2.05	0.62
1:B:311:MET:SD	1:B:326:LEU:HD11	2.40	0.62
1:A:5:ASP:CG	1:A:6:LEU:H	2.06	0.62
1:A:311:MET:SD	1:A:326:LEU:HD11	2.40	0.62
1:B:105:LEU:HD22	1:B:130:SER:HB3	1.82	0.62
1:B:108:GLU:OE2	1:B:127:ASP:OD2	2.18	0.62
1:A:108:GLU:OE2	1:A:127:ASP:OD2	2.18	0.61
1:A:149:LEU:HD12	1:A:149:LEU:O	1.99	0.61
1:B:6:LEU:HG	1:B:6:LEU:O	1.98	0.61
1:B:146:THR:O	1:B:148:LYS:N	2.30	0.61
1:B:365:LEU:HD12	3:B:535:HOH:O	2.00	0.61
1:A:105:LEU:HD22	1:A:130:SER:HB3	1.82	0.61
1:A:146:THR:O	1:A:148:LYS:N	2.30	0.61
1:A:230:THR:HG22	1:A:233:THR:CB	2.29	0.61
1:B:149:LEU:O	1:B:149:LEU:HD12	1.99	0.61
1:B:230:THR:HG22	1:B:233:THR:CB	2.29	0.61
1:A:254:LEU:HD13	1:A:322:ILE:HD11	1.83	0.61
1:B:118:THR:CG2	1:B:198:GLY:CA	2.78	0.61
1:B:254:LEU:HD13	1:B:322:ILE:HD11	1.82	0.61
1:B:311:MET:CE	1:B:326:LEU:O	2.43	0.61
1:A:6:LEU:O	1:A:6:LEU:HG	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HG22	1:B:197:GLY:O	2.01	0.61
1:B:403:ARG:O	1:B:404:VAL:HB	2.00	0.61
1:A:311:MET:CE	1:A:326:LEU:O	2.43	0.61
1:A:344:TYR:C	1:A:345:ASN:HD22	2.07	0.61
1:B:344:TYR:C	1:B:345:ASN:HD22	2.07	0.61
1:A:403:ARG:O	1:A:404:VAL:HB	2.00	0.61
1:A:118:THR:CG2	1:A:198:GLY:CA	2.78	0.61
1:A:275:PHE:CE1	1:A:311:MET:SD	2.93	0.61
1:B:275:PHE:CE1	1:B:311:MET:SD	2.93	0.61
1:A:118:THR:HG22	1:A:197:GLY:O	2.01	0.60
1:B:16:MET:HE3	1:B:351:ARG:HD3	1.81	0.60
1:A:16:MET:HE3	1:A:351:ARG:HD3	1.82	0.60
1:B:313:VAL:CG2	2:B:504:C8E:H102	2.32	0.60
1:B:326:LEU:HD23	2:B:504:C8E:H171	1.84	0.60
1:A:396:ILE:HA	1:A:424:ASN:O	2.02	0.60
1:A:229:LEU:HD23	1:A:229:LEU:N	2.14	0.59
1:B:229:LEU:HD23	1:B:229:LEU:N	2.14	0.59
1:B:396:ILE:HA	1:B:424:ASN:O	2.02	0.59
1:A:90:LEU:HD12	1:A:95:PHE:CE1	2.37	0.59
1:B:82:PRO:C	1:B:83:GLN:HG2	2.27	0.59
1:B:90:LEU:HD12	1:B:95:PHE:CE1	2.37	0.59
1:B:243:THR:HG21	1:B:277:MET:SD	2.42	0.59
1:A:374:LEU:HD21	1:A:420:HIS:CD2	2.38	0.59
1:B:157:LEU:HD12	1:B:158:VAL:N	2.18	0.59
1:A:243:THR:HG23	1:A:277:MET:HB2	1.81	0.59
1:A:351:ARG:NH1	1:A:383:GLU:HB2	2.16	0.59
1:B:59:VAL:HG22	1:B:418:GLN:HG3	1.83	0.59
1:B:351:ARG:NH1	1:B:383:GLU:HB2	2.16	0.59
1:A:59:VAL:HG22	1:A:418:GLN:HG3	1.83	0.59
1:A:157:LEU:HD12	1:A:158:VAL:N	2.18	0.59
1:A:243:THR:HG21	1:A:277:MET:SD	2.43	0.59
1:B:374:LEU:HD21	1:B:420:HIS:CD2	2.38	0.59
1:A:9:TYR:CZ	1:A:136:ARG:NH1	2.69	0.59
1:A:82:PRO:C	1:A:83:GLN:HG2	2.28	0.59
1:B:9:TYR:CZ	1:B:136:ARG:NH1	2.69	0.59
1:B:431:LYS:HD2	1:B:433:PHE:CZ	2.37	0.59
1:A:16:MET:CE	1:A:341:ALA:HB2	2.33	0.59
1:B:16:MET:CE	1:B:341:ALA:HB2	2.33	0.59
1:A:131:ARG:HH11	1:A:133:ILE:HD11	1.67	0.58
1:A:431:LYS:HD2	1:A:433:PHE:CZ	2.37	0.58
1:B:166:LEU:HD23	2:B:504:C8E:H142	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HG23	1:B:277:MET:HB2	1.81	0.58
1:A:46:PHE:HE2	1:A:48:LEU:HD12	1.67	0.58
1:B:131:ARG:HH11	1:B:133:ILE:HD11	1.67	0.58
1:B:46:PHE:HE2	1:B:48:LEU:HD12	1.67	0.58
1:A:237:ALA:C	1:A:238:MET:HE2	2.28	0.58
1:B:237:ALA:C	1:B:238:MET:HE2	2.28	0.58
1:B:312:ASN:HB3	3:B:546:HOH:O	2.02	0.58
1:B:146:THR:O	1:B:148:LYS:HG2	2.03	0.57
1:A:43:GLY:HA2	1:A:435:HIS:HE1	1.68	0.57
1:A:146:THR:O	1:A:148:LYS:HG2	2.03	0.57
1:B:43:GLY:HA2	1:B:435:HIS:HE1	1.68	0.57
1:A:149:LEU:HD12	1:A:149:LEU:C	2.29	0.57
1:B:130:SER:HB2	1:B:369:VAL:HG13	1.87	0.57
1:B:149:LEU:HD12	1:B:149:LEU:C	2.29	0.57
1:A:130:SER:HB2	1:A:369:VAL:HG13	1.87	0.57
1:A:292:ARG:HB3	1:A:343:LYS:HB2	1.86	0.57
1:B:122:ILE:HD12	1:B:122:ILE:N	2.18	0.57
1:B:292:ARG:HB3	1:B:343:LYS:HB2	1.86	0.57
1:A:278:PRO:HG2	1:A:304:TRP:CD2	2.40	0.57
1:B:278:PRO:HG2	1:B:304:TRP:CD2	2.40	0.57
1:A:5:ASP:O	1:A:6:LEU:C	2.48	0.56
1:A:122:ILE:N	1:A:122:ILE:HD12	2.19	0.56
1:A:401:ARG:HB2	1:A:421:SER:CB	2.28	0.56
1:B:5:ASP:O	1:B:6:LEU:C	2.48	0.56
1:B:19:THR:HG23	1:B:23:TYR:OH	2.05	0.56
1:B:378:VAL:O	1:B:398:PHE:HD1	1.87	0.56
1:A:19:THR:HG23	1:A:23:TYR:OH	2.05	0.56
1:A:378:VAL:O	1:A:398:PHE:HD1	1.87	0.56
1:A:119:GLU:O	1:A:197:GLY:HA2	2.05	0.56
1:B:119:GLU:O	1:B:197:GLY:HA2	2.05	0.56
1:B:401:ARG:HB2	1:B:421:SER:CB	2.29	0.56
1:B:266:LEU:HD11	1:B:315:PHE:HE2	1.71	0.56
1:A:266:LEU:HD11	1:A:315:PHE:HE2	1.71	0.56
1:A:227:TYR:O	1:A:234:VAL:HG23	2.06	0.55
1:B:118:THR:CG2	1:B:197:GLY:O	2.54	0.55
1:B:227:TYR:O	1:B:234:VAL:HG23	2.06	0.55
1:B:130:SER:CB	1:B:369:VAL:HG13	2.36	0.55
1:A:29:ALA:HA	1:A:32:SER:OG	2.06	0.55
1:A:254:LEU:HD22	1:A:322:ILE:HD13	1.88	0.55
1:B:29:ALA:HA	1:B:32:SER:OG	2.06	0.55
1:B:120:ASN:ND2	1:B:120:ASN:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:THR:HG23	1:B:148:LYS:CG	2.36	0.55
1:A:118:THR:CG2	1:A:197:GLY:O	2.55	0.55
1:A:146:THR:HG23	1:A:148:LYS:CG	2.36	0.55
1:A:130:SER:CB	1:A:369:VAL:HG13	2.36	0.55
1:A:120:ASN:O	1:A:120:ASN:ND2	2.37	0.54
1:A:204:LEU:HD23	1:A:214:VAL:HG21	1.90	0.54
1:B:254:LEU:HD22	1:B:322:ILE:HD13	1.88	0.54
1:B:204:LEU:HD23	1:B:214:VAL:HG21	1.90	0.54
1:A:146:THR:C	1:A:148:LYS:H	2.15	0.54
1:B:146:THR:C	1:B:148:LYS:H	2.15	0.54
1:B:300:LYS:NZ	3:B:519:HOH:O	2.40	0.54
1:B:148:LYS:HB2	1:B:227:TYR:CE1	2.42	0.54
1:A:148:LYS:HB2	1:A:227:TYR:CE1	2.42	0.54
1:B:46:PHE:CE2	1:B:48:LEU:HD12	2.42	0.54
1:B:183:SER:HB2	3:B:541:HOH:O	2.07	0.54
1:A:46:PHE:CE2	1:A:48:LEU:HD12	2.42	0.53
1:A:386:PHE:CE1	1:A:392:ILE:HD11	2.43	0.53
1:B:302:ALA:HB3	1:B:333:ILE:HG22	1.91	0.53
1:B:340:THR:O	1:B:351:ARG:HA	2.08	0.53
1:B:386:PHE:CE1	1:B:392:ILE:HD11	2.43	0.53
1:A:302:ALA:HB3	1:A:333:ILE:HG22	1.91	0.53
1:A:340:THR:O	1:A:351:ARG:HA	2.09	0.53
1:A:44:ASN:ND2	1:A:89:GLN:H	2.07	0.53
1:A:69:SER:O	1:A:70:SER:HB3	2.08	0.53
1:B:120:ASN:C	1:B:120:ASN:HD22	2.16	0.53
1:A:119:GLU:OE1	1:A:171:SER:OG	2.26	0.53
1:B:44:ASN:ND2	1:B:89:GLN:H	2.07	0.53
1:B:343:LYS:NZ	3:B:536:HOH:O	2.42	0.53
1:B:431:LYS:HD2	1:B:433:PHE:CE1	2.44	0.53
1:A:305:GLY:N	1:A:332:ASP:OD2	2.42	0.53
1:A:6:LEU:O	1:A:7:GLU:CB	2.57	0.53
1:A:431:LYS:HD2	1:A:433:PHE:CE1	2.44	0.53
1:B:6:LEU:O	1:B:7:GLU:CB	2.57	0.53
1:B:305:GLY:N	1:B:332:ASP:OD2	2.42	0.53
1:A:11:ALA:O	1:A:395:ALA:HB2	2.09	0.52
1:B:11:ALA:O	1:B:395:ALA:HB2	2.09	0.52
1:B:16:MET:HE2	1:B:351:ARG:HG2	1.91	0.52
1:B:69:SER:O	1:B:70:SER:HB3	2.08	0.52
1:B:119:GLU:OE1	1:B:171:SER:OG	2.26	0.52
1:A:16:MET:HE2	1:A:351:ARG:HG2	1.91	0.52
1:A:232:ASN:O	1:A:287:HIS:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:HIS:HA	1:A:398:PHE:O	2.09	0.52
1:B:232:ASN:O	1:B:287:HIS:HA	2.10	0.52
1:B:377:HIS:HA	1:B:398:PHE:O	2.09	0.52
1:B:156:ASP:HB2	1:B:220:GLY:C	2.34	0.52
1:A:156:ASP:O	1:A:157:LEU:CB	2.54	0.52
1:A:156:ASP:HB2	1:A:220:GLY:C	2.34	0.52
1:B:156:ASP:O	1:B:157:LEU:CB	2.54	0.52
1:A:131:ARG:NH1	1:A:133:ILE:HD11	2.25	0.52
1:A:349:THR:HB	1:A:383:GLU:HB3	1.92	0.52
1:A:260:ASP:OD1	1:B:188:PRO:HD3	2.09	0.51
1:B:82:PRO:HD2	1:B:101:VAL:HG11	1.91	0.51
1:B:137:ALA:O	1:B:156:ASP:O	2.28	0.51
1:A:82:PRO:HD2	1:A:101:VAL:HG11	1.92	0.51
1:A:114:PHE:O	1:A:117:GLN:HG2	2.10	0.51
1:A:191:ALA:HA	2:A:501:C8E:H52	1.93	0.51
1:A:149:LEU:CD1	1:A:149:LEU:C	2.83	0.51
1:A:311:MET:CE	1:A:328:HIS:ND1	2.74	0.51
1:B:157:LEU:HD22	1:B:219:TRP:HZ3	1.75	0.51
1:B:311:MET:CE	1:B:328:HIS:ND1	2.74	0.51
1:B:349:THR:HB	1:B:383:GLU:HB3	1.92	0.51
1:A:302:ALA:HB3	1:A:333:ILE:HG23	1.93	0.51
1:B:131:ARG:NH1	1:B:133:ILE:HD11	2.26	0.51
1:B:170:SER:HA	1:B:173:VAL:HG22	1.93	0.51
1:A:148:LYS:HD2	3:A:531:HOH:O	2.09	0.51
1:A:157:LEU:HD22	1:A:219:TRP:HZ3	1.75	0.51
1:A:170:SER:HA	1:A:173:VAL:HG22	1.93	0.51
1:B:149:LEU:CD1	1:B:149:LEU:C	2.83	0.51
1:B:114:PHE:O	1:B:117:GLN:HG2	2.11	0.51
1:A:137:ALA:O	1:A:156:ASP:O	2.28	0.51
1:B:302:ALA:HB3	1:B:333:ILE:HG23	1.93	0.51
1:A:212:GLY:O	1:A:213:ALA:CB	2.59	0.51
1:A:230:THR:CG2	1:A:233:THR:CB	2.89	0.51
1:B:16:MET:HE3	1:B:351:ARG:NE	2.26	0.51
1:B:33:ASN:HB2	1:B:238:MET:SD	2.51	0.51
1:B:212:GLY:O	1:B:213:ALA:CB	2.59	0.51
1:B:230:THR:CG2	1:B:233:THR:CB	2.89	0.51
1:A:323:ASP:OD1	1:A:323:ASP:C	2.53	0.51
1:B:35:ALA:HB1	1:B:150:THR:O	2.11	0.51
1:B:203:SER:O	1:B:204:LEU:HD12	2.11	0.51
1:A:35:ALA:HB1	1:A:150:THR:O	2.11	0.50
1:B:323:ASP:C	1:B:323:ASP:OD1	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HE3	1:A:351:ARG:NE	2.26	0.50
1:A:6:LEU:O	1:A:7:GLU:CG	2.59	0.50
1:A:33:ASN:HB2	1:A:238:MET:SD	2.51	0.50
1:A:203:SER:O	1:A:204:LEU:HD12	2.11	0.50
1:A:290:ASN:ND2	1:A:291:GLU:HG2	2.26	0.50
1:B:6:LEU:O	1:B:7:GLU:CG	2.60	0.50
1:B:290:ASN:ND2	1:B:291:GLU:HG2	2.26	0.50
1:B:212:GLY:HA3	1:B:251:LYS:HG2	1.94	0.50
1:B:67:ALA:HB2	1:B:113:SER:OG	2.12	0.50
1:B:131:ARG:HB3	1:B:163:ASN:HB2	1.92	0.50
1:B:167:LEU:HD23	1:B:168:LEU:N	2.26	0.50
1:A:67:ALA:HB2	1:A:113:SER:OG	2.12	0.50
1:A:212:GLY:HA3	1:A:251:LYS:HG2	1.94	0.50
1:A:275:PHE:CZ	1:A:311:MET:CG	2.95	0.50
1:B:328:HIS:O	1:B:329:ARG:CB	2.60	0.50
1:A:328:HIS:O	1:A:329:ARG:CB	2.60	0.50
1:B:146:THR:HG23	1:B:148:LYS:HG3	1.92	0.50
1:B:187:VAL:HB	1:B:188:PRO:CD	2.42	0.50
1:B:275:PHE:CZ	1:B:311:MET:CG	2.95	0.50
1:A:146:THR:HG23	1:A:148:LYS:HG3	1.92	0.49
1:A:187:VAL:HB	1:A:188:PRO:CD	2.42	0.49
1:A:349:THR:HG22	1:A:350:LEU:N	2.26	0.49
1:B:114:PHE:HA	1:B:117:GLN:HG2	1.94	0.49
1:A:167:LEU:HD23	1:A:168:LEU:N	2.27	0.49
1:B:349:THR:HG22	1:B:350:LEU:N	2.26	0.49
1:A:131:ARG:HB3	1:A:163:ASN:HB2	1.92	0.49
1:B:423:ILE:HG22	1:B:424:ASN:N	2.27	0.49
1:A:21:SER:O	1:A:33:ASN:ND2	2.46	0.49
1:A:423:ILE:HG22	1:A:424:ASN:N	2.28	0.49
1:B:175:ALA:O	1:B:179:GLN:CG	2.58	0.49
1:A:106:GLY:HA2	1:A:130:SER:O	2.12	0.49
1:A:114:PHE:HA	1:A:117:GLN:HG2	1.94	0.49
1:A:230:THR:HG21	1:A:233:THR:OG1	2.13	0.49
1:B:21:SER:O	1:B:33:ASN:ND2	2.46	0.49
1:B:313:VAL:HG21	2:B:504:C8E:H102	1.93	0.49
1:A:175:ALA:O	1:A:179:GLN:CG	2.58	0.49
1:B:106:GLY:HA2	1:B:130:SER:O	2.12	0.49
1:A:6:LEU:O	1:A:7:GLU:HG3	2.12	0.49
1:A:345:ASN:HB2	1:A:348:LEU:HB3	1.94	0.49
1:B:6:LEU:O	1:B:7:GLU:HG3	2.12	0.49
1:B:152:GLY:O	1:B:223:LEU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:HG21	1:B:233:THR:OG1	2.13	0.49
1:B:345:ASN:HB2	1:B:348:LEU:HB3	1.95	0.49
1:A:292:ARG:CB	1:A:343:LYS:HB2	2.42	0.48
1:A:344:TYR:CD2	1:A:345:ASN:ND2	2.81	0.48
1:A:396:ILE:HD12	1:A:396:ILE:N	2.28	0.48
1:B:396:ILE:HD12	1:B:396:ILE:N	2.28	0.48
1:B:292:ARG:CB	1:B:343:LYS:HB2	2.42	0.48
1:B:368:PRO:HA	1:B:418:GLN:NE2	2.26	0.48
1:A:152:GLY:O	1:A:223:LEU:HA	2.13	0.48
1:A:368:PRO:HA	1:A:418:GLN:NE2	2.27	0.48
1:B:386:PHE:HE1	1:B:392:ILE:HD11	1.78	0.48
1:B:344:TYR:CD2	1:B:345:ASN:ND2	2.81	0.48
1:A:386:PHE:HE1	1:A:392:ILE:HD11	1.78	0.48
1:B:120:ASN:ND2	1:B:120:ASN:C	2.71	0.48
1:A:120:ASN:ND2	1:A:120:ASN:C	2.71	0.48
1:A:153:ALA:O	1:A:154:SER:HB2	2.13	0.48
1:A:157:LEU:HA	1:A:218:GLY:O	2.13	0.48
1:A:254:LEU:CD2	1:A:322:ILE:HD13	2.43	0.48
1:B:153:ALA:O	1:B:154:SER:HB2	2.13	0.48
1:B:157:LEU:HA	1:B:218:GLY:O	2.13	0.48
1:B:254:LEU:CD2	1:B:322:ILE:HD13	2.43	0.48
1:A:141:PHE:CE2	1:A:153:ALA:HB3	2.48	0.48
1:B:141:PHE:CE2	1:B:153:ALA:HB3	2.48	0.48
1:A:148:LYS:O	1:A:227:TYR:HA	2.14	0.47
1:B:130:SER:OG	1:B:369:VAL:HG13	2.14	0.47
1:A:284:GLY:HA3	1:A:298:ASP:OD2	2.15	0.47
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.79	0.47
1:B:313:VAL:HG22	2:B:504:C8E:H102	1.96	0.47
1:B:90:LEU:HD12	1:B:95:PHE:HE1	1.79	0.47
1:B:118:THR:CG2	1:B:198:GLY:C	2.88	0.47
1:B:148:LYS:O	1:B:227:TYR:HA	2.14	0.47
1:B:398:PHE:CD1	1:B:398:PHE:N	2.82	0.47
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.79	0.47
1:B:284:GLY:HA3	1:B:298:ASP:OD2	2.15	0.47
1:A:90:LEU:HD12	1:A:95:PHE:HE1	1.80	0.47
1:A:311:MET:HE2	1:A:328:HIS:ND1	2.29	0.47
1:B:122:ILE:HD12	1:B:122:ILE:H	1.79	0.47
1:A:118:THR:CG2	1:A:198:GLY:C	2.88	0.47
1:A:266:LEU:HD11	1:A:315:PHE:CE2	2.49	0.47
1:A:398:PHE:CD1	1:A:398:PHE:N	2.82	0.47
1:B:258:SER:OG	1:B:262:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HD11	1:B:315:PHE:CE2	2.49	0.47
1:A:98:GLY:O	1:A:137:ALA:HA	2.14	0.47
1:B:301:ARG:HD2	1:B:333:ILE:O	2.15	0.47
1:B:388:LYS:H	1:B:388:LYS:HD2	1.79	0.47
1:A:130:SER:OG	1:A:369:VAL:HG13	2.15	0.47
1:A:258:SER:OG	1:A:262:ALA:HB3	2.15	0.47
1:A:301:ARG:HD2	1:A:333:ILE:O	2.15	0.47
1:A:431:LYS:HB2	1:A:433:PHE:HE1	1.80	0.47
1:B:379:THR:HG22	1:B:397:SER:HA	1.97	0.47
1:A:312:ASN:O	1:A:313:VAL:HG23	2.14	0.46
1:A:379:THR:HG22	1:A:397:SER:HA	1.98	0.46
1:A:167:LEU:HD23	1:A:167:LEU:C	2.40	0.46
1:A:388:LYS:H	1:A:388:LYS:HD2	1.80	0.46
1:B:431:LYS:HB2	1:B:433:PHE:HE1	1.80	0.46
1:B:41:PRO:HG2	1:B:432:ASN:ND2	2.22	0.46
1:B:98:GLY:O	1:B:137:ALA:HA	2.14	0.46
1:B:312:ASN:O	1:B:313:VAL:HG23	2.15	0.46
1:A:41:PRO:HG2	1:A:432:ASN:ND2	2.23	0.46
1:A:122:ILE:HD12	1:A:122:ILE:H	1.80	0.46
1:A:366:ILE:HG12	1:A:367:LEU:N	2.30	0.46
1:B:167:LEU:HD23	1:B:167:LEU:C	2.41	0.46
1:B:221:GLY:O	1:B:240:ASN:ND2	2.49	0.46
1:B:404:VAL:HG13	1:B:404:VAL:O	2.16	0.46
1:A:120:ASN:C	1:A:120:ASN:HD22	2.17	0.46
1:A:221:GLY:O	1:A:240:ASN:ND2	2.49	0.46
1:A:260:ASP:O	1:B:188:PRO:HG3	2.16	0.46
1:B:366:ILE:HG12	1:B:367:LEU:N	2.30	0.46
1:A:404:VAL:O	1:A:404:VAL:HG13	2.16	0.46
1:A:151:PHE:HD2	1:A:152:GLY:N	2.13	0.46
1:A:433:PHE:N	1:A:433:PHE:CD1	2.84	0.46
1:B:151:PHE:HD2	1:B:152:GLY:N	2.13	0.46
1:B:263:VAL:HG12	1:B:265:PRO:HD3	1.98	0.46
1:B:328:HIS:HB2	1:B:329:ARG:H	1.45	0.45
1:B:369:VAL:HG12	1:B:370:ILE:CD1	2.36	0.45
1:A:369:VAL:HG12	1:A:370:ILE:CD1	2.36	0.45
1:B:21:SER:HA	1:B:238:MET:HE1	1.96	0.45
1:B:433:PHE:N	1:B:433:PHE:CD1	2.85	0.45
1:B:235:LEU:HD23	1:B:285:LEU:CB	2.46	0.45
1:A:21:SER:HA	1:A:238:MET:HE1	1.97	0.45
1:A:235:LEU:HD23	1:A:285:LEU:CB	2.46	0.45
1:A:254:LEU:HD22	1:A:322:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ALA:C	1:A:257:ILE:HG13	2.42	0.45
1:B:12:ILE:HD12	1:B:351:ARG:CZ	2.46	0.45
1:B:237:ALA:HA	1:B:282:THR:O	2.16	0.45
1:A:22:SER:HB3	1:A:236:GLY:HA3	1.99	0.45
1:A:28:ALA:C	1:A:30:LEU:N	2.74	0.45
1:A:237:ALA:HA	1:A:282:THR:O	2.16	0.45
1:A:263:VAL:HG12	1:A:265:PRO:HD3	1.98	0.45
1:A:296:ALA:O	1:A:338:ILE:HA	2.16	0.45
1:B:141:PHE:CD1	1:B:141:PHE:C	2.94	0.45
1:A:12:ILE:HD12	1:A:351:ARG:CZ	2.46	0.45
1:A:141:PHE:CD1	1:A:141:PHE:C	2.94	0.45
1:B:5:ASP:OD2	1:B:6:LEU:N	2.50	0.45
1:A:376:ARG:HB3	1:A:400:LEU:HD12	1.95	0.45
1:A:388:LYS:HB3	1:A:388:LYS:HE3	1.80	0.45
1:B:28:ALA:C	1:B:30:LEU:N	2.74	0.45
1:B:156:ASP:N	1:B:220:GLY:O	2.50	0.45
1:B:376:ARG:HB3	1:B:400:LEU:HD12	1.95	0.45
1:A:5:ASP:OD2	1:A:6:LEU:N	2.50	0.45
1:B:119:GLU:O	1:B:197:GLY:CA	2.65	0.45
1:B:254:LEU:HD22	1:B:322:ILE:HD11	1.97	0.45
1:B:379:THR:HG22	1:B:397:SER:HB2	1.98	0.45
1:A:98:GLY:O	1:A:138:PRO:HD2	2.17	0.44
1:A:148:LYS:CD	3:A:531:HOH:O	2.64	0.44
1:A:156:ASP:N	1:A:220:GLY:O	2.51	0.44
1:A:186:LEU:CD1	1:A:266:LEU:HD21	2.46	0.44
1:B:5:ASP:OD2	1:B:5:ASP:C	2.58	0.44
1:B:98:GLY:O	1:B:138:PRO:HD2	2.17	0.44
1:B:296:ALA:O	1:B:338:ILE:HA	2.17	0.44
1:A:5:ASP:OD2	1:A:5:ASP:C	2.58	0.44
1:A:146:THR:O	1:A:146:THR:HG23	2.17	0.44
1:B:22:SER:HB3	1:B:236:GLY:HA3	1.99	0.44
1:B:146:THR:O	1:B:146:THR:HG23	2.17	0.44
1:B:186:LEU:CD1	1:B:266:LEU:HD21	2.46	0.44
1:B:208:SER:C	1:B:209:THR:HG23	2.43	0.44
1:B:256:ALA:C	1:B:257:ILE:HG13	2.43	0.44
1:B:388:LYS:HB3	1:B:388:LYS:HE3	1.80	0.44
1:A:119:GLU:O	1:A:197:GLY:CA	2.65	0.44
1:A:208:SER:C	1:A:209:THR:HG23	2.43	0.44
1:A:238:MET:HE3	1:A:282:THR:HB	1.98	0.44
1:B:238:MET:HE3	1:B:282:THR:HB	1.98	0.44
1:A:433:PHE:N	1:A:433:PHE:HD1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:HD22	1:B:241:PHE:N	2.16	0.44
1:B:433:PHE:N	1:B:433:PHE:HD1	2.15	0.44
1:A:240:ASN:HD22	1:A:241:PHE:N	2.16	0.44
1:A:379:THR:HG22	1:A:397:SER:HB2	1.99	0.44
1:A:148:LYS:HG3	1:A:149:LEU:H	1.82	0.44
1:B:423:ILE:CG2	1:B:424:ASN:N	2.81	0.44
1:B:431:LYS:NZ	3:B:551:HOH:O	2.50	0.44
1:A:423:ILE:CG2	1:A:424:ASN:N	2.81	0.43
1:B:148:LYS:HG3	1:B:149:LEU:H	1.82	0.43
1:B:117:GLN:HE21	1:B:117:GLN:HB3	1.61	0.43
1:A:118:THR:O	1:A:120:ASN:N	2.51	0.43
1:A:113:SER:OG	1:A:114:PHE:N	2.51	0.43
1:A:328:HIS:HB2	1:A:329:ARG:H	1.45	0.43
1:B:94:ARG:HB2	1:B:142:SER:HB3	2.00	0.43
1:A:94:ARG:HB2	1:A:142:SER:HB3	2.00	0.43
1:A:367:LEU:HD23	1:A:369:VAL:H	1.84	0.43
1:A:12:ILE:HD12	1:A:351:ARG:HE	1.80	0.43
1:B:12:ILE:O	1:B:12:ILE:HG13	2.19	0.43
1:B:186:LEU:HD11	1:B:266:LEU:HD21	2.01	0.43
1:B:208:SER:C	1:B:209:THR:CG2	2.92	0.43
1:A:117:GLN:HE21	1:A:117:GLN:HB3	1.61	0.43
1:A:208:SER:C	1:A:209:THR:CG2	2.92	0.43
1:A:257:ILE:HA	1:A:262:ALA:O	2.18	0.43
1:B:12:ILE:HD12	1:B:351:ARG:HE	1.80	0.43
1:B:24:TYR:CZ	1:B:26:GLY:HA2	2.54	0.43
1:B:187:VAL:HB	1:B:188:PRO:HD3	2.01	0.43
1:B:385:ASP:HB3	1:B:391:ARG:HG2	2.01	0.43
1:A:186:LEU:HD11	1:A:266:LEU:HD21	2.01	0.43
1:A:385:ASP:HB3	1:A:391:ARG:HG2	2.01	0.43
1:A:187:VAL:HB	1:A:188:PRO:HD3	2.01	0.42
1:B:118:THR:O	1:B:120:ASN:N	2.52	0.42
1:B:257:ILE:HA	1:B:262:ALA:O	2.19	0.42
1:B:367:LEU:HA	1:B:368:PRO:HD2	1.85	0.42
1:B:367:LEU:HD23	1:B:369:VAL:H	1.84	0.42
1:A:367:LEU:HD23	1:A:367:LEU:C	2.44	0.42
1:B:113:SER:OG	1:B:114:PHE:N	2.51	0.42
1:B:146:THR:HG22	1:B:149:LEU:CD1	2.48	0.42
1:A:12:ILE:O	1:A:12:ILE:HG13	2.19	0.42
1:A:24:TYR:CZ	1:A:26:GLY:HA2	2.55	0.42
1:A:146:THR:HG22	1:A:149:LEU:CD1	2.48	0.42
1:A:230:THR:CG2	1:A:233:THR:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:CE1	1:A:311:MET:HB3	2.55	0.42
1:A:367:LEU:HA	1:A:368:PRO:HD2	1.85	0.42
1:B:230:THR:CG2	1:B:233:THR:N	2.83	0.42
1:B:367:LEU:HD23	1:B:367:LEU:C	2.45	0.42
1:A:6:LEU:O	1:A:7:GLU:HB2	2.20	0.42
1:B:14:ARG:HD2	1:B:426:VAL:CG2	2.49	0.42
1:B:275:PHE:CE1	1:B:311:MET:HB3	2.55	0.42
1:A:58:LYS:CE	1:A:68:LYS:HD3	2.49	0.42
1:B:6:LEU:O	1:B:7:GLU:HB2	2.20	0.42
1:B:14:ARG:NH2	3:B:548:HOH:O	2.52	0.42
1:B:135:LEU:O	1:B:158:VAL:HA	2.19	0.42
1:B:312:ASN:C	1:B:313:VAL:HG23	2.44	0.42
1:A:312:ASN:C	1:A:313:VAL:HG23	2.44	0.42
1:A:14:ARG:HD2	1:A:426:VAL:CG2	2.50	0.42
1:A:135:LEU:O	1:A:158:VAL:HA	2.20	0.42
1:A:69:SER:O	1:A:70:SER:CB	2.68	0.42
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.90	0.42
1:A:370:ILE:O	1:A:370:ILE:HG22	2.20	0.42
1:B:58:LYS:CE	1:B:68:LYS:HD3	2.50	0.42
1:A:156:ASP:HB2	1:A:220:GLY:O	2.20	0.41
1:A:281:LEU:HD22	1:A:281:LEU:HA	1.96	0.41
1:B:145:ALA:O	1:B:146:THR:HB	2.20	0.41
1:B:281:LEU:HD22	1:B:281:LEU:HA	1.96	0.41
1:A:16:MET:CE	1:A:351:ARG:HG2	2.51	0.41
1:A:210:ALA:C	1:A:212:GLY:N	2.77	0.41
1:A:242:LYS:N	1:A:242:LYS:HD2	2.35	0.41
1:B:16:MET:CE	1:B:351:ARG:HG2	2.51	0.41
1:B:242:LYS:HD2	1:B:242:LYS:N	2.35	0.41
1:A:145:ALA:O	1:A:146:THR:HB	2.20	0.41
1:A:292:ARG:HG3	1:A:292:ARG:NH1	2.35	0.41
1:B:156:ASP:HB2	1:B:220:GLY:O	2.20	0.41
1:B:292:ARG:HG3	1:B:292:ARG:NH1	2.35	0.41
1:B:292:ARG:O	1:B:343:LYS:N	2.35	0.41
1:A:292:ARG:O	1:A:343:LYS:N	2.35	0.41
1:B:69:SER:O	1:B:70:SER:CB	2.68	0.41
1:B:210:ALA:C	1:B:212:GLY:N	2.77	0.41
1:A:235:LEU:HD23	1:A:285:LEU:HB3	2.02	0.41
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.91	0.41
1:A:210:ALA:O	1:A:211:GLY:C	2.63	0.41
1:A:134:VAL:HG22	1:A:160:THR:CG2	2.38	0.41
1:A:311:MET:HE1	1:A:328:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HG23	1:B:198:GLY:C	2.45	0.41
1:B:134:VAL:HG22	1:B:160:THR:CG2	2.38	0.41
1:B:235:LEU:HD23	1:B:285:LEU:HB3	2.02	0.41
1:B:311:MET:HE1	1:B:328:HIS:ND1	2.35	0.41
1:A:58:LYS:HE2	1:A:68:LYS:HD3	2.02	0.41
1:B:122:ILE:N	1:B:122:ILE:CD1	2.84	0.41
1:B:157:LEU:HD22	1:B:219:TRP:CZ3	2.55	0.41
1:B:311:MET:CE	1:B:328:HIS:CE1	2.88	0.41
1:A:146:THR:HG23	1:A:148:LYS:HG2	2.01	0.41
1:A:157:LEU:HD22	1:A:219:TRP:CZ3	2.55	0.41
1:A:311:MET:CE	1:A:328:HIS:CE1	2.88	0.41
1:B:146:THR:HG23	1:B:148:LYS:HG2	2.01	0.41
1:B:210:ALA:O	1:B:211:GLY:C	2.64	0.41
1:B:370:ILE:O	1:B:370:ILE:HG22	2.20	0.41
1:B:379:THR:HG22	1:B:397:SER:CA	2.50	0.41
1:A:122:ILE:N	1:A:122:ILE:CD1	2.84	0.41
1:A:118:THR:HG23	1:A:198:GLY:C	2.46	0.40
1:A:379:THR:HG22	1:A:397:SER:CA	2.50	0.40
1:B:58:LYS:HE2	1:B:68:LYS:HD3	2.03	0.40
1:A:11:ALA:HB3	1:A:393:ASN:HB2	2.04	0.40
1:A:176:LEU:HB3	1:A:182:LEU:HB2	2.01	0.40
1:A:333:ILE:CG1	1:A:334:THR:N	2.82	0.40
1:B:148:LYS:HD2	1:B:227:TYR:HE1	1.87	0.40
1:B:176:LEU:HB3	1:B:182:LEU:HB2	2.02	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	404/439 (92%)	354 (88%)	30 (7%)	20 (5%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	404/439 (92%)	354 (88%)	31 (8%)	19 (5%)	2	2
All	All	808/878 (92%)	708 (88%)	61 (8%)	39 (5%)	2	2

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	70	SER
1	A	210	ALA
1	A	274	ASN
1	A	291	GLU
1	A	328	HIS
1	A	329	ARG
1	A	404	VAL
1	B	7	GLU
1	B	70	SER
1	B	210	ALA
1	B	211	GLY
1	B	274	ASN
1	B	291	GLU
1	B	328	HIS
1	B	329	ARG
1	B	404	VAL
1	A	6	LEU
1	A	20	SER
1	A	120	ASN
1	A	157	LEU
1	A	211	GLY
1	A	313	VAL
1	A	366	ILE
1	A	414	GLU
1	B	6	LEU
1	B	20	SER
1	B	120	ASN
1	B	313	VAL
1	B	366	ILE
1	B	414	GLU
1	A	32	SER
1	A	146	THR
1	A	147	SER
1	B	32	SER
1	B	146	THR

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Mol	Chain	Res	Type
1	B	147	SER
1	B	157	LEU
1	A	119	GLU

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	328/350 (94%)	281 (86%)	47 (14%)	3	6
1	B	328/350 (94%)	281 (86%)	47 (14%)	3	6
All	All	656/700 (94%)	562 (86%)	94 (14%)	3	6

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	6	LEU
1	A	12	ILE
1	A	25	THR
1	A	42	ASP
1	A	52	VAL
1	A	58	LYS
1	A	83	GLN
1	A	103	SER
1	A	105	LEU
1	A	117	GLN
1	A	127	ASP
1	A	130	SER
1	A	131	ARG
1	A	135	LEU
1	A	149	LEU
1	A	157	LEU
1	A	160	THR
1	A	164	LEU
1	A	219	TRP

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Mol	Chain	Res	Type
1	A	223	LEU
1	A	229	LEU
1	A	232	ASN
1	A	238	MET
1	A	242	LYS
1	A	255	SER
1	A	266	LEU
1	A	276	GLU
1	A	281	LEU
1	A	282	THR
1	A	285	LEU
1	A	300	LYS
1	A	306	ASP
1	A	308	MET
1	A	311	MET
1	A	318	GLN
1	A	322	ILE
1	A	326	LEU
1	A	333	ILE
1	A	335	VAL
1	A	340	THR
1	A	369	VAL
1	A	388	LYS
1	A	398	PHE
1	A	413	THR
1	A	424	ASN
1	A	435	HIS
1	B	5	ASP
1	B	6	LEU
1	B	12	ILE
1	B	25	THR
1	B	42	ASP
1	B	52	VAL
1	B	58	LYS
1	B	83	GLN
1	B	103	SER
1	B	105	LEU
1	B	117	GLN
1	B	127	ASP
1	B	130	SER
1	B	131	ARG
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	149	LEU
1	B	157	LEU
1	B	160	THR
1	B	164	LEU
1	B	219	TRP
1	B	223	LEU
1	B	229	LEU
1	B	232	ASN
1	B	238	MET
1	B	242	LYS
1	B	255	SER
1	B	266	LEU
1	B	276	GLU
1	B	281	LEU
1	B	282	THR
1	B	285	LEU
1	B	300	LYS
1	B	306	ASP
1	B	308	MET
1	B	311	MET
1	B	318	GLN
1	B	322	ILE
1	B	326	LEU
1	B	333	ILE
1	B	335	VAL
1	B	340	THR
1	B	369	VAL
1	B	388	LYS
1	B	398	PHE
1	B	413	THR
1	B	424	ASN
1	B	435	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	89	GLN
1	A	117	GLN
1	A	123	GLN
1	A	240	ASN
1	A	287	HIS

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Mol	Chain	Res	Type
1	A	290	ASN
1	A	345	ASN
1	A	358	GLN
1	A	418	GLN
1	A	420	HIS
1	A	424	ASN
1	A	432	ASN
1	A	435	HIS
1	A	436	HIS
1	B	44	ASN
1	B	89	GLN
1	B	117	GLN
1	B	123	GLN
1	B	240	ASN
1	B	287	HIS
1	B	290	ASN
1	B	345	ASN
1	B	358	GLN
1	B	418	GLN
1	B	420	HIS
1	B	424	ASN
1	B	432	ASN
1	B	435	HIS
1	B	436	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	C8E	B	502	-	20,20,20	1.35	3 (15%)	19,19,19	2.39	6 (31%)
2	C8E	A	503	-	20,20,20	1.39	1 (5%)	19,19,19	2.17	6 (31%)
2	C8E	B	504	-	20,20,20	1.12	1 (5%)	19,19,19	2.25	8 (42%)
2	C8E	A	501	-	20,20,20	0.98	0	19,19,19	2.03	6 (31%)

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	C8E	B	502	-	-	10/18/18/18	-
2	C8E	A	503	-	-	10/18/18/18	-
2	C8E	B	504	-	-	8/18/18/18	-
2	C8E	A	501	-	-	8/18/18/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	C8E	O12-C11	2.86	1.54	1.42
2	B	504	C8E	C14-C13	2.49	1.61	1.49
2	B	502	C8E	O18-C19	2.41	1.52	1.42
2	B	502	C8E	C19-C20	2.18	1.61	1.49
2	B	502	C8E	C14-C13	2.12	1.59	1.49

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	C8E	O15-C14-C13	5.41	135.03	110.35
2	B	502	C8E	O15-C14-C13	4.91	132.75	110.35
2	A	501	C8E	O15-C14-C13	4.64	131.49	110.35
2	B	502	C8E	O18-C19-C20	4.54	130.11	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	C8E	O12-C13-C14	4.36	130.23	110.35
2	A	503	C8E	O18-C19-C20	4.11	128.21	110.11
2	A	503	C8E	O15-C14-C13	4.06	128.87	110.35
2	A	503	C8E	C7-C6-C5	-3.92	94.54	114.37
2	A	503	C8E	O18-C17-C16	3.90	128.11	110.35
2	B	504	C8E	O18-C17-C16	3.87	128.01	110.35
2	A	501	C8E	O12-C13-C14	3.55	126.52	110.35
2	B	502	C8E	C7-C6-C5	-3.54	96.49	114.37
2	B	504	C8E	C7-C6-C5	-3.27	97.84	114.37
2	A	501	C8E	C7-C6-C5	-3.22	98.09	114.37
2	B	502	C8E	O18-C17-C16	3.14	124.67	110.35
2	A	501	C8E	O18-C19-C20	3.10	123.79	110.11
2	B	504	C8E	O12-C13-C14	3.04	124.20	110.35
2	B	504	C8E	O18-C19-C20	2.95	123.13	110.11
2	A	501	C8E	O9-C8-C7	2.94	125.74	110.32
2	A	503	C8E	O9-C8-C7	2.93	125.70	110.32
2	B	502	C8E	O9-C8-C7	2.89	125.51	110.32
2	A	501	C8E	O18-C17-C16	2.75	122.86	110.35
2	B	504	C8E	C16-O15-C14	-2.45	102.55	113.26
2	B	504	C8E	O9-C8-C7	2.37	122.75	110.32
2	A	503	C8E	O12-C13-C14	2.22	120.47	110.35
2	B	504	C8E	O12-C11-C10	2.05	119.71	110.35

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	C8E	O15-C16-C17-O18
2	A	501	C8E	O12-C13-C14-O15
2	A	501	C8E	O15-C16-C17-O18
2	B	504	C8E	C6-C7-C8-O9
2	A	503	C8E	C6-C7-C8-O9
2	B	504	C8E	C4-C5-C6-C7
2	A	503	C8E	O18-C19-C20-O21
2	B	504	C8E	O9-C10-C11-O12
2	B	504	C8E	C2-C3-C4-C5
2	B	502	C8E	C5-C6-C7-C8
2	B	502	C8E	C2-C3-C4-C5
2	B	502	C8E	C3-C4-C5-C6
2	B	502	C8E	C4-C5-C6-C7
2	A	501	C8E	C6-C7-C8-O9
2	A	501	C8E	C2-C3-C4-C5

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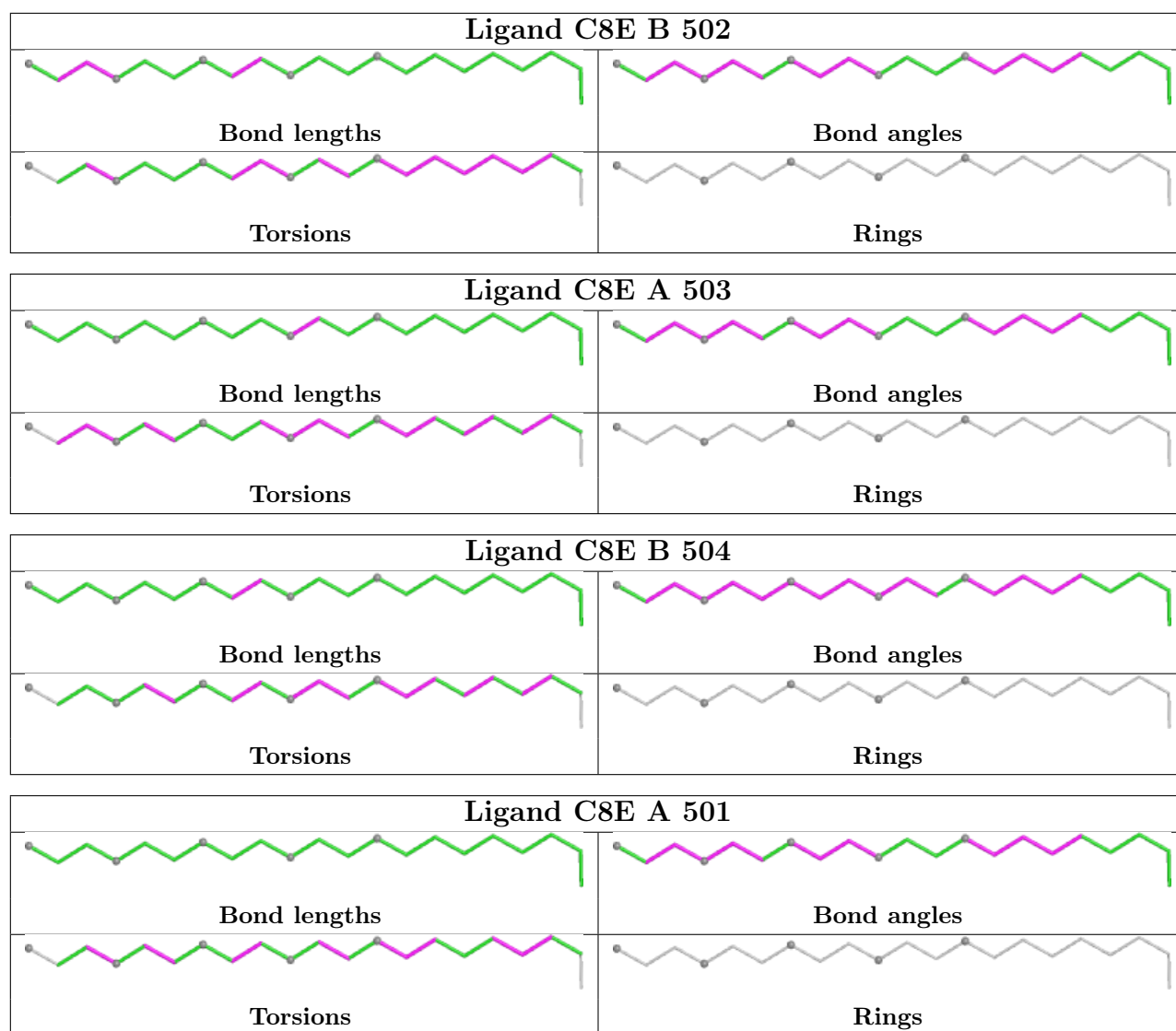
Mol	Chain	Res	Type	Atoms
2	A	503	C8E	O9-C10-C11-O12
2	A	501	C8E	C3-C4-C5-C6
2	B	504	C8E	O12-C13-C14-O15
2	B	502	C8E	C20-C19-O18-C17
2	A	503	C8E	C10-C11-O12-C13
2	B	502	C8E	O9-C10-C11-O12
2	A	503	C8E	C20-C19-O18-C17
2	B	504	C8E	C7-C8-O9-C10
2	B	502	C8E	C14-C13-O12-C11
2	B	502	C8E	O12-C13-C14-O15
2	B	502	C8E	C7-C8-O9-C10
2	A	503	C8E	C4-C5-C6-C7
2	A	501	C8E	C7-C8-O9-C10
2	A	503	C8E	C7-C8-O9-C10
2	B	504	C8E	O15-C16-C17-O18
2	B	504	C8E	C10-C11-O12-C13
2	A	501	C8E	C20-C19-O18-C17
2	B	502	C8E	C6-C7-C8-O9
2	A	501	C8E	O9-C10-C11-O12
2	A	503	C8E	C14-C13-O12-C11
2	A	503	C8E	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	C8E	7	0
2	A	501	C8E	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/439 (94%)	-0.83	0 100 100	24, 46, 81, 98	0
1	B	414/439 (94%)	-0.86	0 100 100	24, 46, 82, 99	0
All	All	828/878 (94%)	-0.84	0 100 100	24, 46, 82, 99	0

There are no RSRZ outliers to report.

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.

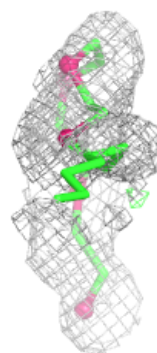
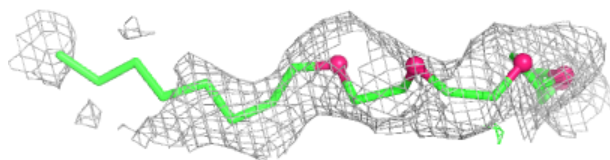
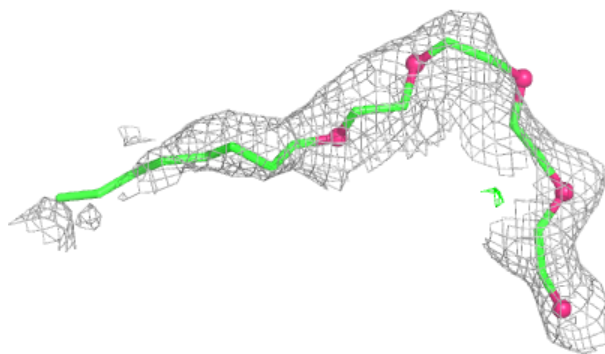
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	C8E	A	503	21/21	0.97	0.07	94,96,96,96	0
2	C8E	B	502	21/21	0.97	0.06	73,86,103,104	6
2	C8E	A	501	21/21	0.98	0.06	71,84,103,105	6
2	C8E	B	504	21/21	0.98	0.07	92,96,99,99	0

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

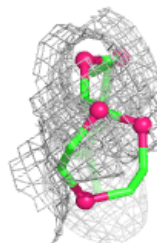
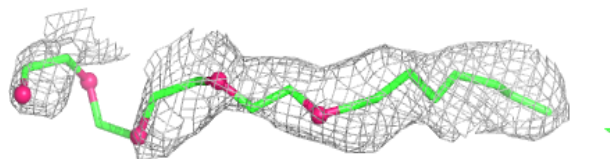
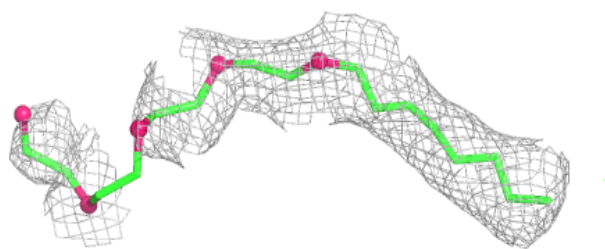
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C8E A 503:

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

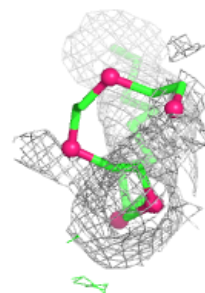
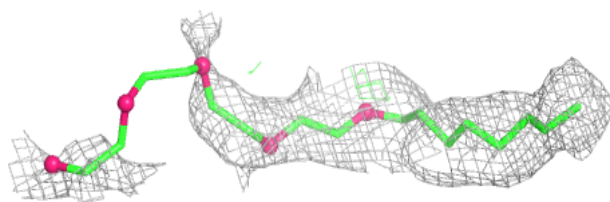
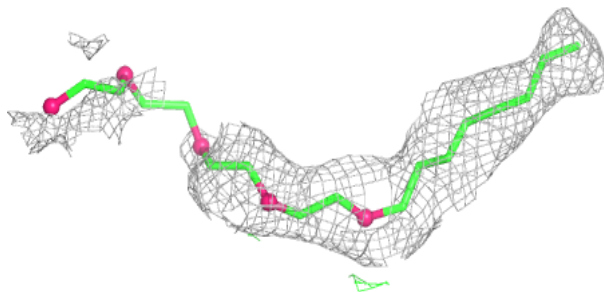
**Electron density around C8E B 502:**

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

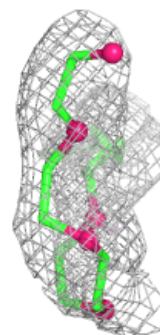
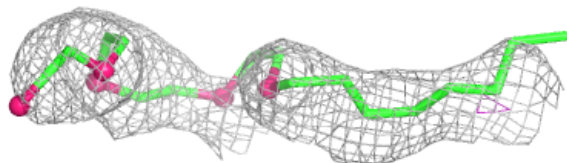
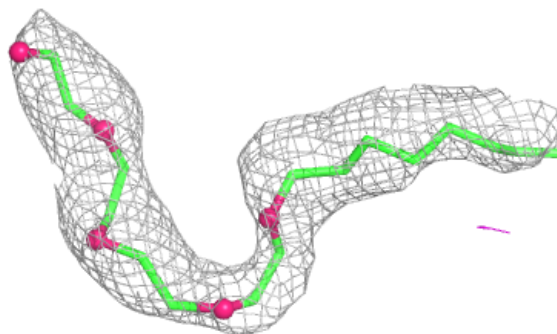


Electron density around C8E A 501:

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

**Electron density around C8E B 504:**

$2mF_o-DF_c$ (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.