WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:40 AM EDT

PDB ID	:	2QTK
Title	:	Crystal Structure of the outer membrane protein opdK from Pseudomonas aeruginosa
Authors	:	Biswas, S.; Van den Berg, B.
Deposited on	:	2007-08-02
Resolution	:	2.80 Å(reported)

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

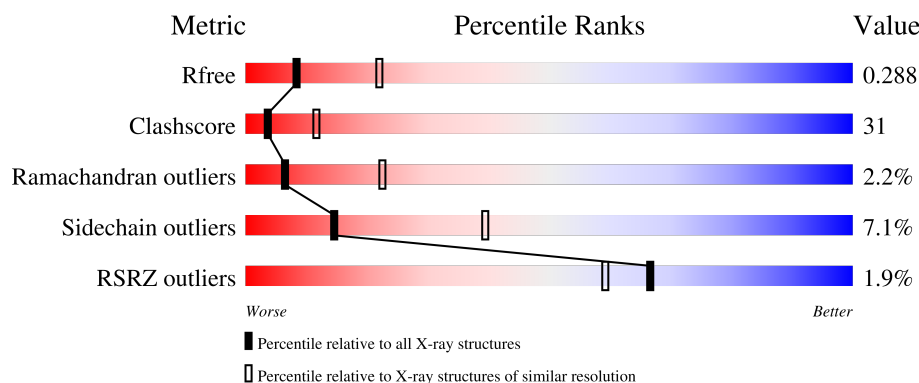|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		31
Ramachandran outliers		2.2%
Sidechain outliers		7.1%
RSRZ outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	390	2% 51% 41% • 5%
1	B	390	2% 48% 40% 6% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	A	393	-	-	-	X
2	C8E	A	395	-	-	-	X
2	C8E	A	400	-	-	-	X
2	C8E	A	401	-	-	-	X
2	C8E	A	402	-	-	-	X
2	C8E	B	396	-	-	-	X
2	C8E	B	399	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6068 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 Probable porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2907	1836	519	547	5			
1	B	368	Total	C	N	O	S	0	0	0
			2888	1825	515	543	5			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).
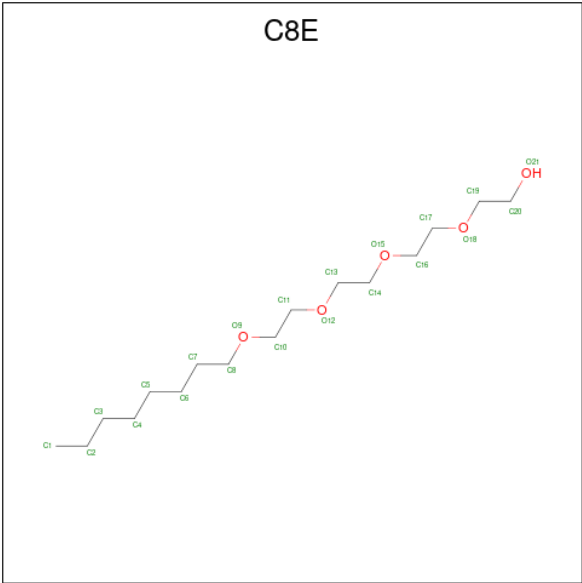
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			15	10	5		
2	A	1	Total	C	O	0	0
			13	11	2		

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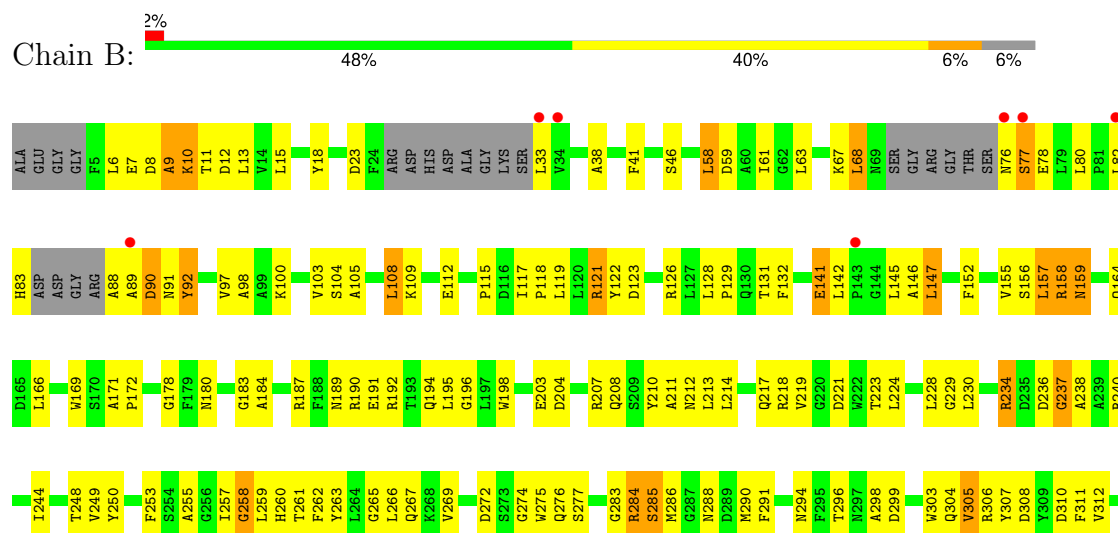| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 17	C 13	O 4	0	0
2	A	1	Total 6	C 6		0	0
2	A	1	Total 9	C 8	O 1	0	0
2	A	1	Total 12	C 10	O 2	0	0
2	A	1	Total 12	C 10	O 2	0	0
2	A	1	Total 12	C 10	O 2	0	0
2	A	1	Total 12	C 10	O 2	0	0
2	A	1	Total 14	C 12	O 2	0	0
2	B	1	Total 20	C 15	O 5	0	0
2	B	1	Total 13	C 8	O 5	0	0
2	B	1	Total 8	C 7	O 1	0	0
2	B	1	Total 12	C 10	O 2	0	0
2	B	1	Total 15	C 12	O 3	0	0
2	B	1	Total 15	C 12	O 3	0	0
2	B	1	Total 9	C 8	O 1	0	0
2	B	1	Total 7	C 7		0	0
2	B	1	Total 13	C 11	O 2	0	0
2	B	1	Total 13	C 11	O 2	0	0

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: Probable porin
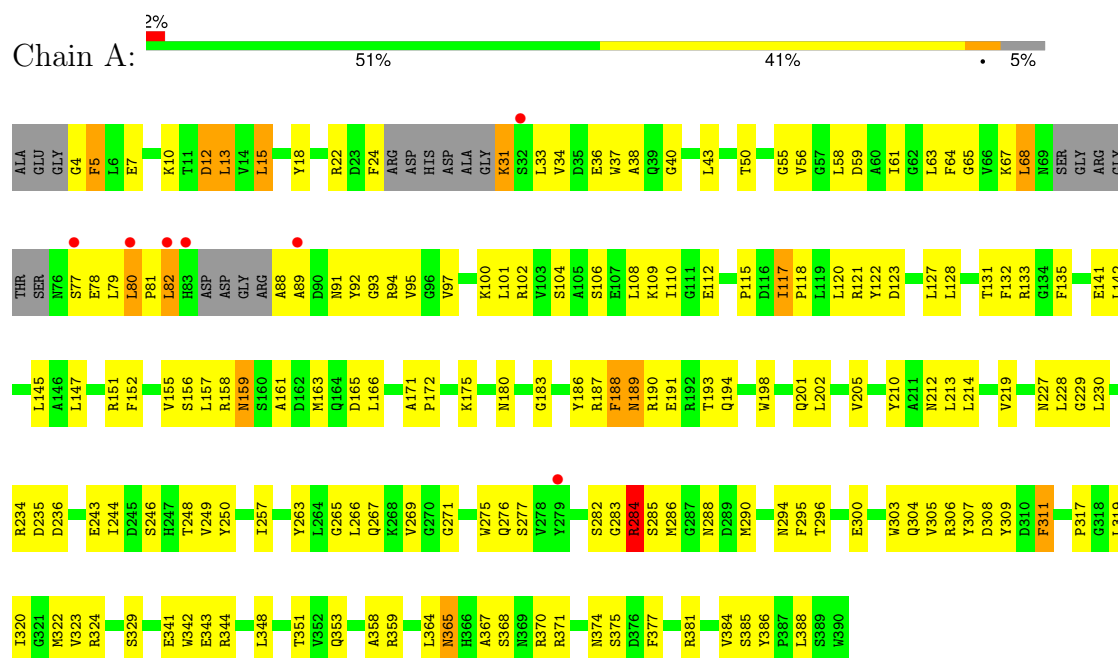
- Molecule 1: Probable porin

P317 G318 L319 I320 G321 M322 V323 R324 Y325 G326 T332 E341 W342 E343 R344 D345 V346 E347 L348 G349 Y350 T351 V352 Q353 S354 A358 R359 V362 R363 L364 N365 H366 A367 S368 N369 R370 R371 S372 R381 V384 S385 Y386 F387 L388 S389 W390

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.89Å　96.70Å　121.41Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	10.00 – 2.80 48.77 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.4 (10.00-2.80) 98.7 (48.77-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233　,　0.295 0.228　,　0.288	Depositor DCC
R_{free} test set	1862 reflections (7.83%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6068	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1285e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

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	0.41	0/2974	0.67	0/4019
1	B	0.41	0/2955	0.66	0/3995
All	All	0.41	0/5929	0.67	0/8014

There are no bond length outliers.

There are no bond angle outliers.

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	2907	0	2782	186	0
1	B	2888	0	2761	192	0
2	A	148	0	237	10	0
2	B	125	0	201	7	0
All	All	6068	0	5981	379	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 31.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:SER:HB3	1:A:82:LEU:HG	1.37	1.02
1:A:13:LEU:HD23	1:A:43:LEU:HD13	1.44	0.98
1:A:365:ASN:HD21	1:A:381:ARG:HD3	1.28	0.97
1:B:142:LEU:HD12	1:B:142:LEU:H	1.28	0.95
1:A:36:GLU:OE1	1:A:78:GLU:HB2	1.72	0.90
1:B:119:LEU:HD22	1:B:208:GLN:HE21	1.37	0.89
1:A:344:ARG:HH11	2:A:392:C8E:H101	1.38	0.88
1:B:77:SER:HB3	1:B:82:LEU:HG	1.55	0.87
1:B:298:ALA:HB3	1:B:332:THR:HG23	1.58	0.85
1:A:159:ASN:H	1:A:159:ASN:HD22	1.22	0.83
1:B:290:MET:HE3	1:B:326:GLY:HA3	1.61	0.83
1:B:155:VAL:CG2	1:B:166:LEU:HG	2.09	0.82
1:B:207:ARG:HE	1:B:234:ARG:HD2	1.44	0.82
1:B:145:LEU:HD21	1:B:147:LEU:HD13	1.59	0.82
1:B:159:ASN:HD22	1:B:159:ASN:H	1.25	0.82
1:A:117:ILE:HD11	1:A:120:LEU:HB3	1.62	0.81
1:B:121:ARG:HD3	1:B:284:ARG:HD2	1.63	0.81
1:B:119:LEU:HD22	1:B:208:GLN:NE2	1.98	0.79
1:B:344:ARG:NH2	1:B:366:HIS:HD2	1.80	0.79
1:B:207:ARG:NE	1:B:234:ARG:HD2	1.97	0.79
1:A:80:LEU:HD23	1:A:81:PRO:HD2	1.64	0.78
1:A:80:LEU:HG	1:A:92:TYR:CE1	2.20	0.77
1:B:145:LEU:CD2	1:B:147:LEU:HD13	2.14	0.76
1:B:155:VAL:HG21	1:B:166:LEU:HG	1.67	0.76
1:B:145:LEU:HD23	1:B:146:ALA:N	2.00	0.76
1:B:204:ASP:HA	1:B:237:GLY:O	1.86	0.76
1:A:371:ARG:HH21	1:A:374:ASN:HD22	1.35	0.75
1:B:142:LEU:H	1:B:142:LEU:CD1	2.01	0.74
1:B:142:LEU:HD12	1:B:142:LEU:N	2.02	0.73
1:B:299:ASP:OD2	1:B:332:THR:HG21	1.89	0.72
1:B:323:VAL:HG12	1:B:346:VAL:HG22	1.70	0.71
1:A:290:MET:HE1	1:A:343:GLU:HB3	1.72	0.71
1:B:159:ASN:HD22	1:B:159:ASN:N	1.84	0.71
1:B:344:ARG:HH22	1:B:366:HIS:HD2	1.37	0.71
1:A:159:ASN:HD22	1:A:159:ASN:N	1.85	0.70
1:A:344:ARG:NH1	2:A:392:C8E:H101	2.06	0.70
1:A:13:LEU:CD2	1:A:43:LEU:HD13	2.21	0.70
1:A:267:GLN:HE22	1:A:286:MET:HG3	1.54	0.70
1:A:290:MET:CE	1:A:343:GLU:HB3	2.21	0.70
1:B:157:LEU:HD22	1:B:164:GLN:HE22	1.56	0.70
1:A:132:PHE:CD1	1:A:155:VAL:HG12	2.26	0.70
1:A:31:LYS:HZ1	1:A:34:VAL:HG23	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASN:H	1:A:159:ASN:ND2	1.88	0.70
1:A:121:ARG:HD3	1:A:284:ARG:HD2	1.73	0.69
1:A:31:LYS:HE2	1:A:33:LEU:H	1.58	0.69
1:B:230:LEU:HD13	1:B:249:VAL:HG12	1.74	0.69
1:A:304:GLN:HG2	1:A:305:VAL:N	2.07	0.68
1:B:121:ARG:HB3	1:B:284:ARG:NH1	2.08	0.68
1:A:219:VAL:HG23	1:A:219:VAL:O	1.94	0.68
1:A:306:ARG:HG3	1:A:324:ARG:HB3	1.76	0.68
1:B:131:THR:HG22	1:B:156:SER:HB3	1.75	0.68
1:B:306:ARG:HG3	1:B:324:ARG:HB3	1.76	0.68
1:A:386:TYR:HE1	1:A:388:LEU:HG	1.58	0.67
1:A:10:LYS:HG3	1:A:12:ASP:OD1	1.93	0.67
1:A:365:ASN:C	1:A:365:ASN:HD22	1.98	0.67
1:B:67:LYS:HB2	1:B:80:LEU:CD1	2.24	0.67
1:B:219:VAL:HG23	1:B:219:VAL:O	1.95	0.67
1:B:105:ALA:HB3	1:B:141:GLU:OE2	1.94	0.67
1:A:133:ARG:HB2	1:A:163:MET:HE1	1.76	0.66
1:A:155:VAL:HG11	1:A:166:LEU:HG	1.76	0.66
1:A:77:SER:HB2	1:A:80:LEU:O	1.95	0.66
1:B:159:ASN:H	1:B:159:ASN:ND2	1.90	0.66
1:B:344:ARG:HD2	2:B:391:C8E:H41	1.78	0.66
1:B:265:GLY:O	1:B:303:TRP:HA	1.95	0.65
1:B:58:LEU:HD23	1:B:58:LEU:C	2.17	0.65
1:A:358:ALA:O	1:A:359:ARG:HB2	1.96	0.65
1:B:365:ASN:C	1:B:365:ASN:HD22	2.01	0.65
1:A:371:ARG:HH21	1:A:374:ASN:ND2	1.96	0.64
1:A:189:ASN:OD1	1:A:190:ARG:N	2.30	0.64
1:B:131:THR:CG2	1:B:156:SER:HB3	2.28	0.64
1:B:320:ILE:HG22	1:B:321:GLY:N	2.12	0.64
1:B:237:GLY:O	1:B:238:ALA:HB3	1.97	0.64
1:B:299:ASP:HB2	1:B:332:THR:HG22	1.80	0.64
1:B:218:ARG:HG3	1:B:218:ARG:HH11	1.63	0.63
1:B:323:VAL:HG11	2:B:391:C8E:H81	1.79	0.63
1:A:58:LEU:HD11	1:A:97:VAL:HG13	1.79	0.63
1:A:59:ASP:OD2	1:A:100:LYS:HD3	1.98	0.63
1:A:67:LYS:HB2	1:A:80:LEU:HD13	1.81	0.63
1:A:67:LYS:NZ	1:A:88:ALA:HB1	2.14	0.63
1:A:228:LEU:HB3	2:A:398:C8E:H51	1.80	0.62
1:A:155:VAL:CG1	1:A:166:LEU:HG	2.28	0.62
1:B:283:GLY:O	1:B:285:SER:N	2.32	0.62
1:A:311:PHE:HB2	1:A:319:LEU:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD23	1:B:146:ALA:H	1.65	0.62
1:B:77:SER:CB	1:B:82:LEU:HG	2.29	0.61
1:B:221:ASP:HB3	1:B:257:ILE:CD1	2.30	0.61
1:B:290:MET:CE	1:B:326:GLY:HA3	2.29	0.61
1:A:290:MET:HE2	1:A:295:PHE:CE1	2.36	0.61
1:B:8:ASP:O	1:B:9:ALA:HB2	2.00	0.61
1:B:67:LYS:HD3	1:B:89:ALA:O	2.01	0.61
1:B:132:PHE:CD1	1:B:155:VAL:HG22	2.36	0.61
1:B:352:VAL:HG12	1:B:358:ALA:HA	1.83	0.60
1:B:221:ASP:HB3	1:B:257:ILE:HD13	1.84	0.60
1:B:304:GLN:HG2	1:B:305:VAL:N	2.16	0.60
1:A:55:GLY:O	1:A:101:LEU:HA	2.02	0.60
1:A:275:TRP:HB3	1:A:296:THR:HB	1.84	0.60
1:B:298:ALA:CB	1:B:332:THR:HG23	2.29	0.60
1:B:228:LEU:HB3	2:B:400:C8E:H111	1.84	0.59
2:A:391:C8E:H172	2:A:399:C8E:H102	1.84	0.59
1:B:298:ALA:O	1:B:332:THR:HG22	2.01	0.59
1:A:133:ARG:HB2	1:A:163:MET:CE	2.33	0.58
1:A:80:LEU:HD23	1:A:81:PRO:CD	2.34	0.58
1:B:261:THR:HB	1:B:308:ASP:HB2	1.86	0.58
1:A:50:THR:OG1	1:A:56:VAL:HG22	2.02	0.58
1:A:151:ARG:HD2	1:A:180:ASN:ND2	2.17	0.58
1:A:230:LEU:HD13	1:A:249:VAL:HG12	1.86	0.58
1:B:67:LYS:HB2	1:B:80:LEU:HD11	1.85	0.58
1:B:344:ARG:HH22	1:B:366:HIS:CD2	2.20	0.58
1:A:10:LYS:HE2	1:A:12:ASP:CG	2.24	0.57
1:B:10:LYS:O	1:B:10:LYS:HD3	2.03	0.57
1:B:123:ASP:OD1	1:B:158:ARG:NH1	2.36	0.57
1:A:267:GLN:HE22	1:A:288:ASN:H	1.52	0.57
1:B:157:LEU:HD22	1:B:164:GLN:NE2	2.19	0.57
1:B:229:GLY:HA3	1:B:250:TYR:CE2	2.39	0.57
1:A:65:GLY:O	1:A:91:ASN:HB2	2.04	0.57
1:A:117:ILE:CD1	1:A:120:LEU:HB3	2.35	0.57
1:B:122:TYR:O	1:B:284:ARG:NH2	2.38	0.56
1:B:342:TRP:CZ2	1:B:370:ARG:HG3	2.40	0.56
1:A:267:GLN:NE2	1:A:288:ASN:H	2.03	0.56
1:A:322:MET:HG2	1:A:323:VAL:N	2.19	0.56
1:B:187:ARG:NH2	1:B:194:GLN:NE2	2.53	0.56
1:A:117:ILE:O	1:A:121:ARG:HG2	2.06	0.56
1:A:61:ILE:HG12	1:A:63:LEU:HD21	1.88	0.56
1:B:67:LYS:HB2	1:B:80:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:LEU:CD1	1:B:249:VAL:HG12	2.36	0.56
1:A:31:LYS:HE2	1:A:33:LEU:N	2.20	0.56
1:A:117:ILE:HD13	1:A:120:LEU:O	2.04	0.55
1:B:178:GLY:O	1:B:203:GLU:HG3	2.06	0.55
1:B:105:ALA:HB3	1:B:141:GLU:CD	2.27	0.55
1:A:165:ASP:HB2	1:A:175:LYS:HD2	1.87	0.55
1:B:92:TYR:OH	1:B:128:LEU:HD23	2.06	0.55
1:A:37:TRP:CE3	1:A:68:LEU:HD12	2.41	0.55
1:A:186:TYR:CE2	1:A:188:PHE:HB3	2.41	0.55
1:B:253:PHE:HZ	2:B:394:C8E:H61	1.71	0.55
1:A:18:TYR:CD2	1:A:79:LEU:HD21	2.41	0.55
1:A:344:ARG:HH11	1:A:344:ARG:HG3	1.72	0.55
1:A:121:ARG:HB3	1:A:284:ARG:NH1	2.22	0.55
1:B:59:ASP:OD2	1:B:100:LYS:HD3	2.07	0.55
1:A:31:LYS:NZ	1:A:34:VAL:HG23	2.21	0.54
1:A:40:GLY:N	1:A:127:LEU:HD11	2.22	0.54
1:A:386:TYR:CE1	1:A:388:LEU:HG	2.41	0.54
1:B:263:TYR:HB2	1:B:306:ARG:HB3	1.88	0.54
1:A:351:THR:HG21	1:A:359:ARG:HH21	1.73	0.54
1:A:265:GLY:O	1:A:303:TRP:HA	2.08	0.54
1:B:145:LEU:HD21	1:B:147:LEU:CD1	2.32	0.54
1:B:267:GLN:HB3	1:B:288:ASN:HD22	1.73	0.54
1:B:189:ASN:O	1:B:190:ARG:HG2	2.08	0.53
1:A:67:LYS:HZ3	1:A:88:ALA:HB1	1.73	0.53
1:A:92:TYR:CZ	1:A:128:LEU:HD23	2.43	0.53
1:B:155:VAL:HG23	1:B:166:LEU:HG	1.88	0.53
1:B:307:TYR:HB3	1:B:323:VAL:HG23	1.90	0.53
1:A:263:TYR:HB2	1:A:306:ARG:HB3	1.89	0.53
1:B:189:ASN:O	1:B:192:ARG:HG2	2.08	0.53
1:B:237:GLY:O	1:B:238:ALA:CB	2.57	0.53
1:A:101:LEU:O	1:A:101:LEU:HD12	2.09	0.53
1:B:306:ARG:HD3	1:B:322:MET:HG3	1.91	0.53
1:A:117:ILE:HD13	1:A:117:ILE:H	1.70	0.53
1:B:91:ASN:O	1:B:92:TYR:HB3	2.08	0.53
1:B:155:VAL:HG23	1:B:166:LEU:CD1	2.39	0.53
1:A:24:PHE:CD1	1:A:377:PHE:HB3	2.43	0.53
1:A:365:ASN:ND2	1:A:381:ARG:HD3	2.11	0.53
1:A:319:LEU:HD11	1:A:348:LEU:HD22	1.91	0.53
1:B:97:VAL:HG12	1:B:98:ALA:N	2.24	0.53
1:A:300:GLU:OE2	1:A:341:GLU:OE1	2.26	0.52
1:A:61:ILE:CD1	1:A:63:LEU:HD21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLN:O	1:A:277:SER:HB3	2.09	0.52
1:A:306:ARG:HD3	1:A:308:ASP:OD1	2.09	0.52
1:B:207:ARG:HG3	1:B:234:ARG:HG3	1.92	0.52
1:B:15:LEU:O	1:B:385:SER:HA	2.10	0.52
1:A:269:VAL:HG21	1:A:296:THR:HA	1.91	0.52
1:B:115:PRO:HG3	1:B:152:PHE:CZ	2.45	0.52
1:A:188:PHE:O	1:A:189:ASN:HB3	2.10	0.52
1:B:103:VAL:O	1:B:104:SER:HB3	2.10	0.52
1:B:112:GLU:OE1	1:B:131:THR:HG21	2.10	0.52
1:B:190:ARG:HD3	1:B:192:ARG:HH21	1.73	0.52
1:B:10:LYS:HD3	1:B:10:LYS:C	2.29	0.51
1:A:93:GLY:O	1:A:161:ALA:HB1	2.10	0.51
1:A:157:LEU:HB3	1:A:159:ASN:ND2	2.25	0.51
1:B:118:PRO:HB3	1:B:210:TYR:CE2	2.45	0.51
1:B:184:ALA:O	1:B:196:GLY:HA2	2.11	0.51
1:B:255:ALA:HB3	1:B:262:PHE:HB2	1.93	0.51
1:A:187:ARG:O	1:A:188:PHE:CD1	2.64	0.51
1:A:306:ARG:HG2	1:A:307:TYR:N	2.25	0.51
1:A:351:THR:HG21	1:A:359:ARG:NH2	2.26	0.51
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.75	0.51
1:B:210:TYR:CZ	1:B:212:ASN:HB2	2.45	0.51
1:B:224:LEU:HD23	2:B:395:C8E:H61	1.91	0.51
1:A:213:LEU:HD12	1:A:214:LEU:N	2.25	0.51
1:A:257:ILE:HG23	1:A:257:ILE:O	2.10	0.51
1:B:218:ARG:HG3	1:B:218:ARG:NH1	2.25	0.51
1:B:364:LEU:HD23	1:B:365:ASN:N	2.25	0.51
1:B:240:ARG:HH11	1:B:240:ARG:HG3	1.75	0.51
1:B:68:LEU:HD12	1:B:68:LEU:O	2.11	0.50
1:B:207:ARG:CD	1:B:234:ARG:HD2	2.40	0.50
1:B:121:ARG:HB3	1:B:284:ARG:HH11	1.77	0.50
1:B:207:ARG:NH1	1:B:236:ASP:OD1	2.44	0.50
1:A:323:VAL:HG11	2:A:392:C8E:H41	1.93	0.50
1:A:92:TYR:OH	1:A:128:LEU:HD23	2.11	0.50
1:A:95:VAL:HG23	2:A:396:C8E:H51	1.93	0.50
1:B:46:SER:HA	1:B:59:ASP:OD1	2.11	0.50
1:B:320:ILE:CG2	1:B:321:GLY:N	2.74	0.50
1:B:219:VAL:O	1:B:219:VAL:CG2	2.59	0.50
1:A:265:GLY:C	1:A:266:LEU:HD12	2.32	0.49
1:A:365:ASN:HD21	1:A:381:ARG:HB2	1.76	0.49
1:B:207:ARG:HE	1:B:234:ARG:NH1	2.09	0.49
1:B:224:LEU:N	1:B:224:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HD23	1:B:109:LYS:N	2.27	0.49
1:A:365:ASN:ND2	1:A:381:ARG:HB2	2.28	0.49
1:A:94:ARG:HG3	1:A:94:ARG:HH11	1.78	0.49
1:B:41:PHE:N	1:B:41:PHE:CD1	2.80	0.49
1:B:155:VAL:HG12	1:B:156:SER:N	2.28	0.49
1:B:386:TYR:HE1	1:B:388:LEU:HG	1.78	0.49
1:B:97:VAL:HG12	1:B:98:ALA:H	1.77	0.48
1:B:159:ASN:N	1:B:159:ASN:ND2	2.53	0.48
1:B:195:LEU:HD21	1:B:213:LEU:HD13	1.95	0.48
1:B:67:LYS:HE2	1:B:88:ALA:HB1	1.94	0.48
1:B:105:ALA:HB3	1:B:141:GLU:HA	1.95	0.48
1:A:159:ASN:N	1:A:159:ASN:ND2	2.53	0.48
1:A:267:GLN:NE2	1:A:286:MET:HG3	2.26	0.48
1:B:126:ARG:HG3	1:B:158:ARG:NE	2.29	0.48
1:B:263:TYR:CD1	1:B:306:ARG:HD2	2.48	0.48
1:B:6:LEU:O	1:B:7:GLU:C	2.51	0.48
1:B:100:LYS:HG2	1:B:109:LYS:HG2	1.95	0.48
1:A:131:THR:CG2	1:A:156:SER:HB3	2.43	0.48
1:B:258:GLY:C	1:B:260:HIS:H	2.16	0.48
1:A:108:LEU:CD2	1:A:110:ILE:HG13	2.43	0.48
1:A:309:TYR:O	1:A:320:ILE:HG13	2.14	0.48
1:B:267:GLN:HB3	1:B:288:ASN:ND2	2.29	0.48
1:A:131:THR:HG22	1:A:156:SER:HB3	1.94	0.48
1:B:258:GLY:O	1:B:260:HIS:N	2.47	0.48
1:B:354:SER:C	1:B:358:ALA:HB2	2.34	0.48
1:B:10:LYS:HG2	1:B:11:THR:N	2.29	0.48
1:A:122:TYR:O	1:A:284:ARG:NH2	2.47	0.47
1:A:121:ARG:HB3	1:A:284:ARG:HH11	1.77	0.47
1:A:151:ARG:CD	1:A:180:ASN:ND2	2.78	0.47
1:A:4:GLY:O	1:A:7:GLU:N	2.47	0.47
1:A:38:ALA:CB	1:A:127:LEU:HD22	2.45	0.47
1:A:290:MET:HE2	1:A:295:PHE:CZ	2.48	0.47
1:B:207:ARG:CG	1:B:234:ARG:HD2	2.44	0.47
1:A:210:TYR:CZ	1:A:212:ASN:HB2	2.49	0.47
1:B:240:ARG:HG3	1:B:240:ARG:NH1	2.30	0.47
1:B:298:ALA:O	1:B:332:THR:CG2	2.63	0.47
1:A:108:LEU:HD23	1:A:109:LYS:N	2.30	0.47
1:A:290:MET:HE2	1:A:295:PHE:HE1	1.79	0.47
1:B:365:ASN:ND2	1:B:381:ARG:HB2	2.30	0.47
1:B:145:LEU:CD2	1:B:146:ALA:N	2.77	0.47
1:B:352:VAL:CG1	1:B:358:ALA:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HG	1:A:92:TYR:HE1	1.72	0.47
1:A:151:ARG:HE	1:A:180:ASN:HD21	1.63	0.47
1:A:282:SER:OG	1:A:284:ARG:HB3	2.16	0.46
1:A:228:LEU:N	1:A:228:LEU:CD1	2.78	0.46
1:A:307:TYR:CD2	2:A:394:C8E:H111	2.51	0.46
1:B:306:ARG:HD3	1:B:308:ASP:OD1	2.16	0.46
1:A:246:SER:HA	1:A:271:GLY:HA3	1.97	0.46
1:B:92:TYR:CZ	1:B:128:LEU:HD23	2.50	0.46
1:A:112:GLU:OE1	1:A:131:THR:HG21	2.15	0.46
1:B:218:ARG:CG	1:B:223:THR:HG23	2.46	0.46
1:A:38:ALA:HB1	1:A:127:LEU:HD22	1.98	0.46
1:B:386:TYR:CE1	1:B:388:LEU:HG	2.51	0.46
1:A:193:THR:HG22	1:A:194:GLN:N	2.30	0.46
1:B:224:LEU:HD12	1:B:224:LEU:H	1.81	0.46
1:B:323:VAL:HG22	2:B:392:C8E:H201	1.97	0.46
1:A:31:LYS:HE3	1:A:33:LEU:O	2.16	0.46
1:B:126:ARG:HB2	1:B:158:ARG:HD3	1.97	0.45
1:A:229:GLY:HA3	1:A:250:TYR:CE2	2.52	0.45
1:B:207:ARG:HE	1:B:234:ARG:CD	2.21	0.45
1:B:311:PHE:HB2	1:B:319:LEU:O	2.15	0.45
1:A:190:ARG:O	1:A:191:GLU:HB2	2.16	0.45
1:B:61:ILE:HD11	1:B:63:LEU:HD21	1.98	0.45
1:B:90:ASP:N	1:B:90:ASP:OD2	2.49	0.45
1:A:171:ALA:N	1:A:172:PRO:HD3	2.32	0.45
1:B:291:PHE:CE1	1:B:345:ASP:HB3	2.51	0.45
1:A:359:ARG:CZ	1:A:359:ARG:HA	2.46	0.45
1:A:343:GLU:HA	1:A:368:SER:O	2.17	0.45
1:B:365:ASN:HD21	1:B:381:ARG:HB2	1.81	0.45
1:A:104:SER:HG	1:A:141:GLU:CD	2.19	0.45
1:A:248:THR:HG21	1:A:286:MET:HE1	1.97	0.45
1:B:76:ASN:O	1:B:77:SER:O	2.35	0.45
1:B:117:ILE:HB	1:B:118:PRO:HD2	1.97	0.44
1:B:276:GLN:O	1:B:277:SER:HB2	2.17	0.44
1:A:214:LEU:HD23	1:A:227:ASN:HA	2.00	0.44
1:B:8:ASP:O	1:B:9:ALA:CB	2.64	0.44
1:A:115:PRO:HG3	1:A:152:PHE:CZ	2.52	0.44
1:B:260:HIS:ND1	1:B:307:TYR:OH	2.50	0.44
1:A:135:PHE:CE2	2:A:395:C8E:H141	2.52	0.44
1:A:234:ARG:HA	1:A:244:ILE:O	2.17	0.44
1:B:38:ALA:HA	1:B:68:LEU:HG	1.99	0.44
1:B:275:TRP:HB3	1:B:296:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:O	1:B:258:GLY:O	2.36	0.44
1:A:13:LEU:HD12	1:A:15:LEU:CD1	2.47	0.44
1:A:235:ASP:HB3	1:A:244:ILE:HB	1.99	0.44
1:A:186:TYR:CZ	1:A:188:PHE:HB3	2.53	0.44
1:A:61:ILE:HD11	1:A:63:LEU:HD21	2.00	0.44
1:B:117:ILE:HB	1:B:118:PRO:CD	2.48	0.44
1:A:193:THR:HG22	1:A:194:GLN:H	1.82	0.43
1:B:80:LEU:HD23	1:B:92:TYR:CE1	2.53	0.43
1:B:303:TRP:HZ3	1:B:305:VAL:HG22	1.83	0.43
1:A:290:MET:HE3	1:A:343:GLU:HB3	1.96	0.43
1:A:300:GLU:HA	1:A:329:SER:O	2.19	0.43
1:A:359:ARG:HH11	1:A:359:ARG:HG2	1.83	0.43
1:A:365:ASN:C	1:A:365:ASN:ND2	2.68	0.43
1:A:22:ARG:HG3	1:A:377:PHE:CD2	2.53	0.43
1:A:344:ARG:O	1:A:367:ALA:HA	2.17	0.43
1:B:108:LEU:HD12	2:B:396:C8E:H71	2.00	0.43
1:B:341:GLU:OE2	1:B:371:ARG:HD2	2.18	0.43
1:A:235:ASP:OD2	1:A:243:GLU:HA	2.19	0.43
1:B:250:TYR:CD1	1:B:250:TYR:C	2.91	0.43
1:B:269:VAL:O	1:B:299:ASP:HA	2.19	0.43
1:A:118:PRO:HB3	1:A:210:TYR:CE2	2.54	0.43
1:A:202:LEU:HD23	1:A:205:VAL:HG11	1.99	0.43
1:A:93:GLY:O	1:A:94:ARG:HB2	2.18	0.43
1:A:145:LEU:HD13	1:A:145:LEU:C	2.38	0.43
1:A:10:LYS:HE2	1:A:12:ASP:OD1	2.18	0.43
1:A:31:LYS:CE	1:A:33:LEU:H	2.29	0.43
1:A:37:TRP:CD2	1:A:68:LEU:HD11	2.54	0.43
1:A:151:ARG:NE	1:A:180:ASN:HD21	2.17	0.43
1:A:155:VAL:HG13	1:A:166:LEU:CD1	2.48	0.43
1:B:310:ASP:HA	1:B:320:ILE:HD13	2.01	0.43
1:A:61:ILE:CG1	1:A:63:LEU:HD21	2.48	0.42
1:A:101:LEU:HD12	1:A:101:LEU:C	2.40	0.42
1:B:304:GLN:CG	1:B:305:VAL:N	2.83	0.42
1:B:306:ARG:CG	1:B:324:ARG:HB3	2.45	0.42
1:B:365:ASN:HD21	1:B:381:ARG:HD3	1.82	0.42
1:A:228:LEU:N	1:A:228:LEU:HD12	2.35	0.42
1:A:229:GLY:HA3	1:A:250:TYR:CZ	2.55	0.42
1:B:183:GLY:HA3	1:B:198:TRP:CE3	2.55	0.42
1:A:187:ARG:O	1:A:188:PHE:O	2.38	0.42
1:A:304:GLN:CG	1:A:305:VAL:N	2.80	0.42
1:B:190:ARG:O	1:B:191:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:LEU:C	1:B:364:LEU:CD2	2.88	0.42
1:A:22:ARG:HG3	1:A:377:PHE:HD2	1.84	0.42
1:B:180:ASN:ND2	1:B:203:GLU:OE2	2.53	0.42
1:B:213:LEU:O	1:B:214:LEU:HD23	2.20	0.42
1:A:151:ARG:HD2	1:A:180:ASN:HD21	1.85	0.42
1:A:187:ARG:HA	1:A:194:GLN:HG3	2.02	0.42
1:A:187:ARG:O	1:A:193:THR:O	2.38	0.42
1:A:342:TRP:CZ2	1:A:370:ARG:HG3	2.55	0.42
1:B:10:LYS:HE3	1:B:12:ASP:OD1	2.19	0.41
1:B:63:LEU:HD22	1:B:129:PRO:HD2	2.01	0.41
1:B:274:GLY:O	1:B:276:GLN:NE2	2.52	0.41
1:B:365:ASN:C	1:B:365:ASN:ND2	2.68	0.41
1:A:351:THR:O	1:A:353:GLN:NE2	2.50	0.41
1:A:13:LEU:HD22	1:A:13:LEU:HA	1.92	0.41
1:A:151:ARG:CD	1:A:180:ASN:HD21	2.33	0.41
1:B:77:SER:HB3	1:B:82:LEU:CG	2.39	0.41
1:B:155:VAL:HG23	1:B:166:LEU:CG	2.51	0.41
1:A:94:ARG:HG3	1:A:94:ARG:NH1	2.35	0.41
1:A:102:ARG:HG2	1:A:106:SER:O	2.19	0.41
1:B:343:GLU:HA	1:B:368:SER:O	2.20	0.41
1:A:283:GLY:O	1:A:285:SER:N	2.53	0.41
1:B:310:ASP:C	1:B:312:VAL:H	2.23	0.41
1:A:123:ASP:OD1	1:A:158:ARG:HD3	2.21	0.41
1:A:384:VAL:HG21	2:A:391:C8E:H191	2.02	0.41
1:B:204:ASP:O	1:B:240:ARG:HG2	2.20	0.41
1:B:211:ALA:HB3	1:B:230:LEU:HB3	2.02	0.41
1:B:244:ILE:HD13	1:B:276:GLN:CD	2.40	0.41
1:A:4:GLY:O	1:A:5:PHE:C	2.59	0.41
1:A:102:ARG:HB3	1:A:102:ARG:CZ	2.50	0.41
1:A:341:GLU:CB	1:A:371:ARG:HG3	2.51	0.41
1:A:235:ASP:OD2	1:A:244:ILE:N	2.42	0.41
1:A:374:ASN:CG	1:A:375:SER:H	2.24	0.41
1:B:169:TRP:O	1:B:172:PRO:HD3	2.21	0.41
1:B:218:ARG:HG2	1:B:223:THR:HG23	2.03	0.41
1:B:248:THR:HG21	1:B:286:MET:CE	2.51	0.41
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.93	0.41
1:B:358:ALA:O	1:B:359:ARG:CB	2.69	0.41
1:B:362:VAL:HG22	1:B:384:VAL:HG22	2.02	0.41
1:B:171:ALA:N	1:B:172:PRO:HD3	2.36	0.41
1:B:219:VAL:HG22	1:B:224:LEU:CD1	2.51	0.41
1:A:67:LYS:O	1:A:68:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:HD13	1:B:350:TYR:HB2	2.03	0.40
1:A:183:GLY:HA3	1:A:198:TRP:CE3	2.56	0.40
1:A:15:LEU:O	1:A:385:SER:HA	2.22	0.40
1:A:61:ILE:HG12	1:A:63:LEU:CD2	2.51	0.40
1:B:58:LEU:C	1:B:58:LEU:CD2	2.88	0.40
1:A:4:GLY:N	1:A:7:GLU:HB2	2.36	0.40
1:A:64:PHE:HB2	2:A:396:C8E:H32	2.02	0.40
1:A:201:GLN:HE21	1:A:236:ASP:CG	2.25	0.40
1:B:33:LEU:C	1:B:33:LEU:HD12	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	363/390 (93%)	319 (88%)	37 (10%)	7 (2%)	8	26
1	B	360/390 (92%)	320 (89%)	31 (9%)	9 (2%)	5	19
All	All	723/780 (93%)	639 (88%)	68 (9%)	16 (2%)	6	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	89	ALA
1	A	188	PHE
1	B	9	ALA
1	B	77	SER
1	B	237	GLY
1	B	258	GLY
1	B	284	ARG
1	A	311	PHE

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Mol	Chain	Res	Type
1	A	317	PRO
1	A	189	ASN
1	A	284	ARG
1	B	141	GLU
1	B	259	LEU
1	B	317	PRO
1	B	78	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	297/309 (96%)	282 (95%)	15 (5%)	24	55
1	B	295/309 (96%)	268 (91%)	27 (9%)	9	27
All	All	592/618 (96%)	550 (93%)	42 (7%)	14	39

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	13	LEU
1	A	15	LEU
1	A	31	LYS
1	A	68	LEU
1	A	80	LEU
1	A	82	LEU
1	A	117	ILE
1	A	142	LEU
1	A	147	LEU
1	A	159	ASN
1	A	284	ARG
1	A	294	ASN
1	A	364	LEU
1	A	365	ASN
1	B	10	LYS

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Mol	Chain	Res	Type
1	B	13	LEU
1	B	18	TYR
1	B	23	ASP
1	B	58	LEU
1	B	68	LEU
1	B	83	HIS
1	B	90	ASP
1	B	92	TYR
1	B	108	LEU
1	B	121	ARG
1	B	147	LEU
1	B	157	LEU
1	B	158	ARG
1	B	159	ASN
1	B	217	GLN
1	B	234	ARG
1	B	266	LEU
1	B	272	ASP
1	B	285	SER
1	B	294	ASN
1	B	305	VAL
1	B	323	VAL
1	B	332	THR
1	B	364	LEU
1	B	365	ASN
1	B	372	SER

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

Mol	Chain	Res	Type
1	A	159	ASN
1	A	164	GLN
1	A	180	ASN
1	A	208	GLN
1	A	267	GLN
1	A	288	ASN
1	A	297	ASN
1	A	304	GLN
1	A	365	ASN
1	A	374	ASN
1	B	21	ASN
1	B	159	ASN

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Mol	Chain	Res	Type
1	B	164	GLN
1	B	174	GLN
1	B	189	ASN
1	B	194	GLN
1	B	201	GLN
1	B	208	GLN
1	B	215	HIS
1	B	288	ASN
1	B	294	ASN
1	B	304	GLN
1	B	330	ASN
1	B	353	GLN
1	B	365	ASN
1	B	366	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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	397	-	8,8,20	0.81	0	7,7,19	1.50	2 (28%)
2	C8E	A	401	-	11,11,20	0.71	0	10,10,19	1.65	2 (20%)
2	C8E	B	392	-	12,12,20	0.98	0	11,11,19	2.20	4 (36%)
2	C8E	B	395	-	14,14,20	0.83	0	13,13,19	1.93	4 (30%)
2	C8E	B	398	-	6,6,20	0.81	0	5,5,19	1.08	0
2	C8E	B	396	-	14,14,20	0.75	0	13,13,19	1.94	4 (30%)
2	C8E	A	397	-	8,8,20	0.84	0	7,7,19	1.53	2 (28%)
2	C8E	A	394	-	12,12,20	0.77	0	11,11,19	1.48	2 (18%)
2	C8E	B	399	-	12,12,20	0.70	0	11,11,19	1.48	2 (18%)
2	C8E	A	399	-	11,11,20	0.76	0	10,10,19	1.60	2 (20%)
2	C8E	A	400	-	11,11,20	0.72	0	10,10,19	1.57	2 (20%)
2	C8E	B	391	-	19,19,20	0.95	0	18,18,19	2.13	6 (33%)
2	C8E	A	393	-	14,14,20	0.81	0	13,13,19	1.97	4 (30%)
2	C8E	A	392	-	12,12,20	0.77	0	11,11,19	1.49	2 (18%)
2	C8E	B	394	-	11,11,20	0.51	0	10,10,19	1.46	2 (20%)
2	C8E	B	393	-	7,7,20	0.76	0	6,6,19	1.61	2 (33%)
2	C8E	A	402	-	13,13,20	0.78	0	12,12,19	1.53	2 (16%)
2	C8E	A	395	-	16,16,20	0.87	0	15,15,19	2.04	4 (26%)
2	C8E	A	398	-	11,11,20	0.71	0	10,10,19	1.55	2 (20%)
2	C8E	A	396	-	5,5,20	0.74	0	4,4,19	0.63	0
2	C8E	A	391	-	12,12,20	0.92	0	11,11,19	2.24	4 (36%)
2	C8E	B	400	-	12,12,20	0.87	0	11,11,19	1.38	2 (18%)

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.

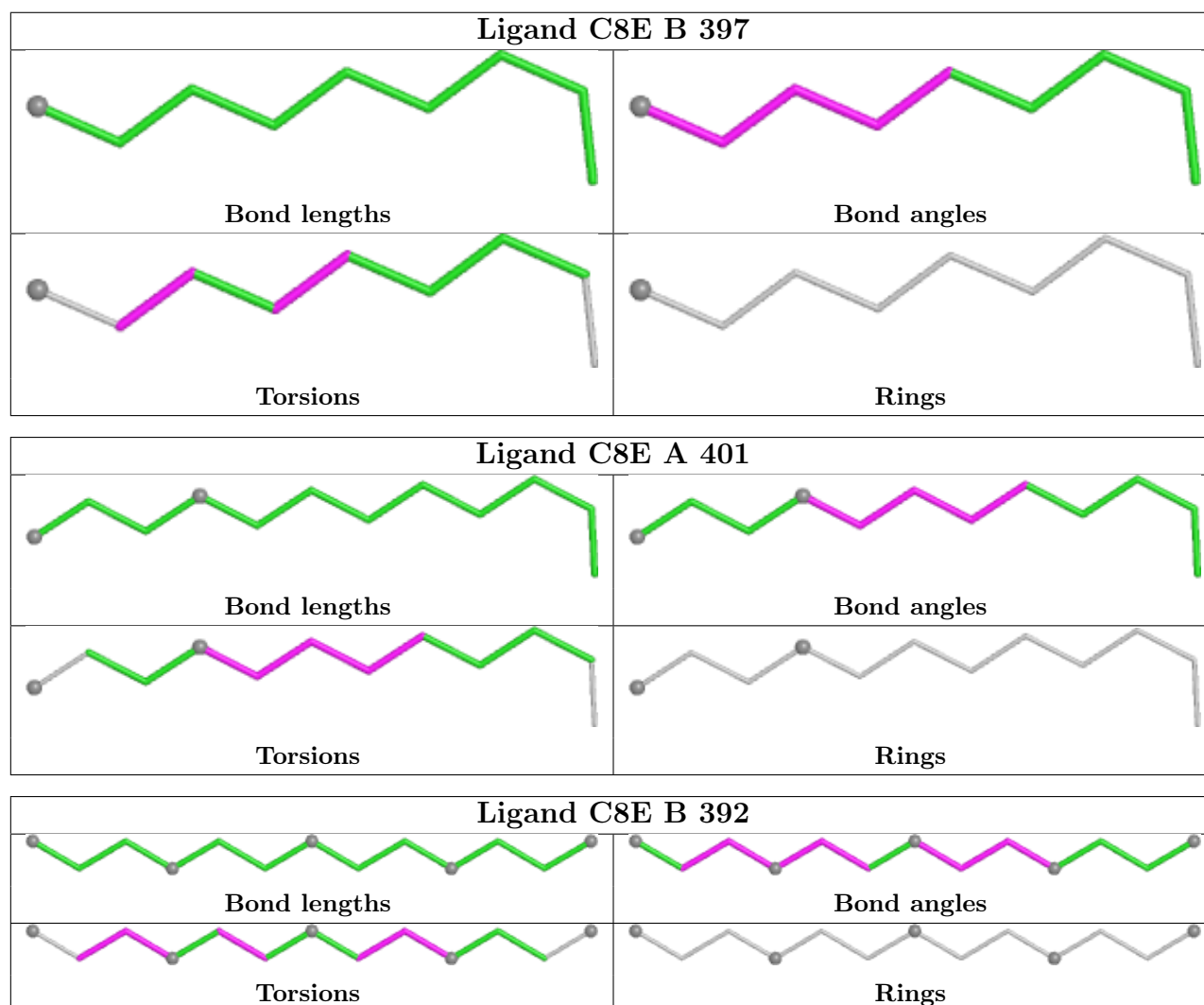| Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	B	397	-	-	2/6/6/18	-
2	C8E	A	401	-	-	4/9/9/18	-
2	C8E	B	392	-	-	5/10/10/18	-
2	C8E	B	395	-	-	8/12/12/18	-
2	C8E	B	398	-	-	3/4/4/18	-
2	C8E	B	396	-	-	4/12/12/18	-
2	C8E	A	397	-	-	2/6/6/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	A	394	-	-	6/10/10/18	-
2	C8E	B	399	-	-	8/10/10/18	-
2	C8E	A	399	-	-	7/9/9/18	-
2	C8E	A	400	-	-	3/9/9/18	-
2	C8E	B	391	-	-	7/17/17/18	-
2	C8E	A	393	-	-	5/12/12/18	-
2	C8E	A	392	-	-	7/10/10/18	-
2	C8E	B	394	-	-	6/9/9/18	-
2	C8E	B	393	-	-	3/5/5/18	-
2	C8E	A	402	-	-	7/11/11/18	-
2	C8E	A	395	-	-	8/14/14/18	-
2	C8E	A	398	-	-	4/9/9/18	-
2	C8E	A	396	-	-	2/3/3/18	-
2	C8E	A	391	-	-	5/10/10/18	-
2	C8E	B	400	-	-	5/10/10/18	-

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	391	C8E	O15-C14-C13	5.03	133.26	110.35
2	A	391	C8E	O15-C14-C13	4.76	132.03	110.35
2	A	395	C8E	O15-C14-C13	4.53	131.01	110.35
2	B	392	C8E	O15-C14-C13	4.52	130.93	110.35
2	A	393	C8E	O15-C14-C13	4.15	129.28	110.35
2	B	395	C8E	O12-C13-C14	3.61	126.03	110.11
2	B	394	C8E	O9-C8-C7	3.53	128.84	110.32
2	B	396	C8E	O9-C8-C7	3.50	128.72	110.32
2	B	392	C8E	O12-C13-C14	3.47	126.15	110.35
2	B	391	C8E	O12-C13-C14	3.46	126.13	110.35
2	A	401	C8E	O9-C8-C7	3.43	128.35	110.32
2	A	395	C8E	O12-C13-C14	3.40	125.84	110.35
2	A	399	C8E	O9-C8-C7	3.31	127.69	110.32
2	A	402	C8E	O9-C8-C7	3.30	127.67	110.32
2	B	396	C8E	O12-C13-C14	3.29	124.62	110.11
2	B	396	C8E	O15-C14-C13	3.25	130.95	111.82
2	B	399	C8E	O9-C8-C7	3.24	127.35	110.32
2	B	395	C8E	O9-C8-C7	3.24	127.31	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	391	C8E	O12-C13-C14	3.24	125.10	110.35
2	A	392	C8E	O9-C8-C7	3.22	127.22	110.32
2	A	393	C8E	O12-C13-C14	3.21	124.98	110.35
2	B	391	C8E	O18-C17-C16	3.20	124.95	110.35
2	A	400	C8E	O9-C8-C7	3.18	127.03	110.32
2	B	395	C8E	O15-C14-C13	3.18	130.54	111.82
2	A	395	C8E	O9-C8-C7	3.18	127.01	110.32
2	A	394	C8E	O9-C8-C7	3.16	126.89	110.32
2	A	398	C8E	O9-C8-C7	3.15	126.85	110.32
2	A	391	C8E	O18-C19-C20	3.08	123.67	110.11
2	B	391	C8E	O9-C8-C7	3.07	126.42	110.32
2	A	395	C8E	C7-C6-C5	-3.03	99.07	114.37
2	B	400	C8E	O9-C8-C7	3.01	126.12	110.32
2	B	391	C8E	O18-C19-C20	3.00	123.34	110.11
2	A	391	C8E	O18-C17-C16	2.96	123.83	110.35
2	B	392	C8E	O18-C19-C20	2.94	123.08	110.11
2	B	396	C8E	C7-C6-C5	-2.94	99.52	114.37
2	A	398	C8E	C7-C6-C5	-2.93	99.57	114.37
2	B	393	C8E	C7-C6-C5	-2.92	99.61	114.37
2	B	392	C8E	O18-C17-C16	2.92	123.66	110.35
2	A	393	C8E	O18-C19-C20	2.91	122.95	110.11
2	B	391	C8E	C7-C6-C5	-2.87	99.85	114.37
2	A	400	C8E	C7-C6-C5	-2.87	99.86	114.37
2	A	399	C8E	C7-C6-C5	-2.86	99.93	114.37
2	A	401	C8E	C7-C6-C5	-2.80	100.23	114.37
2	B	397	C8E	C7-C6-C5	-2.80	100.23	114.37
2	A	402	C8E	C7-C6-C5	-2.78	100.31	114.37
2	A	397	C8E	C7-C6-C5	-2.77	100.38	114.37
2	B	399	C8E	C7-C6-C5	-2.76	100.39	114.37
2	A	394	C8E	C7-C6-C5	-2.68	100.81	114.37
2	A	392	C8E	C7-C6-C5	-2.60	101.25	114.37
2	B	394	C8E	C7-C6-C5	-2.52	101.63	114.37
2	B	395	C8E	C7-C6-C5	-2.51	101.68	114.37
2	A	393	C8E	O18-C17-C16	2.48	121.66	110.35
2	B	400	C8E	C7-C6-C5	-2.48	101.84	114.37
2	A	397	C8E	O9-C8-C7	2.38	126.53	111.44
2	B	393	C8E	O9-C8-C7	2.21	125.51	111.44
2	B	397	C8E	O9-C8-C7	2.16	125.14	111.44

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	395	C8E	O12-C13-C14-O15
2	B	392	C8E	O15-C16-C17-O18
2	A	400	C8E	C6-C7-C8-O9
2	A	391	C8E	O9-C10-C11-O12
2	A	401	C8E	C6-C7-C8-O9
2	A	393	C8E	O9-C10-C11-O12
2	A	394	C8E	C6-C7-C8-O9
2	B	395	C8E	C6-C7-C8-O9
2	B	400	C8E	C6-C7-C8-O9
2	A	393	C8E	O18-C19-C20-O21
2	B	391	C8E	O18-C19-C20-O21
2	B	392	C8E	O12-C13-C14-O15
2	B	396	C8E	C6-C7-C8-O9
2	B	394	C8E	C5-C6-C7-C8
2	A	402	C8E	C2-C3-C4-C5
2	A	402	C8E	C4-C5-C6-C7
2	B	399	C8E	C3-C4-C5-C6
2	B	400	C8E	C4-C5-C6-C7
2	B	394	C8E	C3-C4-C5-C6
2	A	399	C8E	C5-C6-C7-C8
2	A	392	C8E	C5-C6-C7-C8
2	B	393	C8E	C5-C6-C7-C8
2	A	399	C8E	O9-C10-C11-O12
2	B	394	C8E	O9-C10-C11-O12
2	B	399	C8E	C6-C7-C8-O9
2	B	399	C8E	C5-C6-C7-C8
2	B	395	C8E	C4-C5-C6-C7
2	B	391	C8E	C6-C7-C8-O9
2	A	391	C8E	O12-C13-C14-O15
2	B	391	C8E	O12-C13-C14-O15
2	B	398	C8E	C2-C3-C4-C5
2	B	395	C8E	C2-C3-C4-C5
2	B	391	C8E	C5-C6-C7-C8
2	B	396	C8E	O9-C10-C11-O12
2	A	393	C8E	C14-C13-O12-C11
2	A	397	C8E	C6-C7-C8-O9
2	B	395	C8E	C3-C4-C5-C6
2	B	400	C8E	O9-C10-C11-O12
2	A	395	C8E	O9-C10-C11-O12
2	A	394	C8E	C2-C3-C4-C5
2	B	400	C8E	C3-C4-C5-C6
2	A	399	C8E	C4-C5-C6-C7
2	A	395	C8E	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	B	399	C8E	C1-C2-C3-C4
2	A	394	C8E	C4-C5-C6-C7
2	B	393	C8E	C2-C3-C4-C5
2	B	398	C8E	C4-C5-C6-C7
2	A	399	C8E	C1-C2-C3-C4
2	A	391	C8E	O18-C19-C20-O21
2	B	397	C8E	C4-C5-C6-C7
2	B	393	C8E	C4-C5-C6-C7
2	B	399	C8E	C4-C5-C6-C7
2	B	391	C8E	C4-C5-C6-C7
2	A	394	C8E	C1-C2-C3-C4
2	A	395	C8E	C3-C4-C5-C6
2	A	392	C8E	C1-C2-C3-C4
2	B	394	C8E	C2-C3-C4-C5
2	A	397	C8E	C5-C6-C7-C8
2	A	392	C8E	C4-C5-C6-C7
2	A	393	C8E	C7-C8-O9-C10
2	A	392	C8E	C10-C11-O12-C13
2	A	398	C8E	C1-C2-C3-C4
2	A	396	C8E	C3-C4-C5-C6
2	A	402	C8E	C10-C11-O12-C13
2	A	401	C8E	C5-C6-C7-C8
2	B	392	C8E	C20-C19-O18-C17
2	A	391	C8E	C14-C13-O12-C11
2	A	391	C8E	C20-C19-O18-C17
2	B	392	C8E	C14-C13-O12-C11
2	A	401	C8E	C4-C5-C6-C7
2	A	395	C8E	C14-C13-O12-C11
2	A	402	C8E	C3-C4-C5-C6
2	A	398	C8E	O9-C10-C11-O12
2	A	394	C8E	C3-C4-C5-C6
2	A	392	C8E	C6-C7-C8-O9
2	B	399	C8E	C10-C11-O12-C13
2	B	400	C8E	C7-C8-O9-C10
2	A	399	C8E	C6-C7-C8-O9
2	A	399	C8E	C3-C4-C5-C6
2	B	396	C8E	C3-C4-C5-C6
2	B	394	C8E	C7-C8-O9-C10
2	A	400	C8E	C7-C8-O9-C10
2	B	391	C8E	C7-C8-O9-C10
2	A	393	C8E	O12-C13-C14-O15
2	A	402	C8E	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	398	C8E	C7-C8-O9-C10
2	A	401	C8E	C7-C8-O9-C10
2	A	402	C8E	C7-C8-O9-C10
2	B	395	C8E	C7-C8-O9-C10
2	B	399	C8E	C7-C8-O9-C10
2	A	392	C8E	C7-C8-O9-C10
2	A	394	C8E	C7-C8-O9-C10
2	A	395	C8E	C7-C8-O9-C10
2	A	399	C8E	C7-C8-O9-C10
2	B	396	C8E	C7-C8-O9-C10
2	A	398	C8E	C2-C3-C4-C5
2	B	395	C8E	O9-C10-C11-O12
2	B	398	C8E	C1-C2-C3-C4
2	A	395	C8E	C10-C11-O12-C13
2	A	402	C8E	C14-C13-O12-C11
2	A	395	C8E	C4-C5-C6-C7
2	B	394	C8E	C6-C7-C8-O9
2	B	395	C8E	C10-C11-O12-C13
2	A	396	C8E	C2-C3-C4-C5
2	A	400	C8E	C2-C3-C4-C5
2	B	397	C8E	C6-C7-C8-O9
2	B	395	C8E	O12-C13-C14-O15
2	B	399	C8E	O9-C10-C11-O12
2	B	392	C8E	O18-C19-C20-O21
2	A	392	C8E	O9-C10-C11-O12
2	B	391	C8E	O9-C10-C11-O12

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	392	C8E	1	0
2	B	395	C8E	1	0
2	B	396	C8E	1	0
2	A	394	C8E	1	0
2	A	399	C8E	1	0
2	B	391	C8E	2	0
2	A	392	C8E	3	0
2	B	394	C8E	1	0
2	A	395	C8E	1	0
2	A	398	C8E	1	0
2	A	396	C8E	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	391	C8E	2	0
2	B	400	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand C8E B 397

Bond lengths   Bond angles

Torsions   Rings

Ligand C8E A 401

Bond lengths   Bond angles

Torsions   Rings

Ligand C8E B 392

Bond lengths   Bond angles

Torsions   Rings

Ligand C8E B 395

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 398

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 396

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 397

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 394

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 399

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 399

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 400

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 391

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 393

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 392

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 394

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 393

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 395

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 398

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 396

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 391

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E B 400	
Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	371/390 (95%)	-0.04	7 (1%)	66	59	14, 29, 50, 69	0
1	B	368/390 (94%)	-0.07	7 (1%)	66	59	15, 29, 53, 73	0
All	All	739/780 (94%)	-0.06	14 (1%)	66	59	14, 29, 51, 73	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	SER	7.0
1	A	77	SER	4.4
1	B	33	LEU	3.3
1	B	76	ASN	3.0
1	B	82	LEU	2.9
1	B	34	VAL	2.7
1	B	89	ALA	2.7
1	A	279	TYR	2.6
1	A	83	HIS	2.6
1	A	82	LEU	2.4
1	A	32	SER	2.4
1	B	143	PRO	2.3
1	A	80	LEU	2.3
1	A	89	ALA	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	402	14/21	0.44	0.74	67,71,74,74	0
2	C8E	A	401	12/21	0.56	0.48	63,73,74,74	0
2	C8E	A	400	12/21	0.60	0.56	61,66,67,67	0
2	C8E	A	395	17/21	0.64	0.66	59,71,73,73	0
2	C8E	B	399	13/21	0.65	0.42	52,64,68,68	0
2	C8E	A	399	12/21	0.71	0.32	51,53,58,59	0
2	C8E	B	391	20/21	0.73	0.38	41,57,63,64	0
2	C8E	B	396	15/21	0.75	0.61	63,65,70,70	0
2	C8E	A	398	12/21	0.75	0.34	51,56,59,59	0
2	C8E	B	394	12/21	0.76	0.32	61,66,69,69	0
2	C8E	A	393	15/21	0.78	0.44	43,54,59,60	0
2	C8E	B	397	9/21	0.80	0.31	64,66,68,68	0
2	C8E	B	395	15/21	0.81	0.38	66,72,73,74	0
2	C8E	B	392	13/21	0.81	0.40	61,66,69,69	0
2	C8E	B	400	13/21	0.82	0.47	73,76,79,79	0
2	C8E	A	396	6/21	0.86	0.23	44,45,46,46	0
2	C8E	A	397	9/21	0.87	0.27	44,46,51,52	0
2	C8E	B	398	7/21	0.87	0.22	54,56,57,58	0
2	C8E	A	394	13/21	0.87	0.26	39,41,50,51	0
2	C8E	B	393	8/21	0.87	0.25	52,54,55,55	0
2	C8E	A	392	13/21	0.89	0.27	39,46,49,49	0
2	C8E	A	391	13/21	0.90	0.28	49,51,54,54	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.
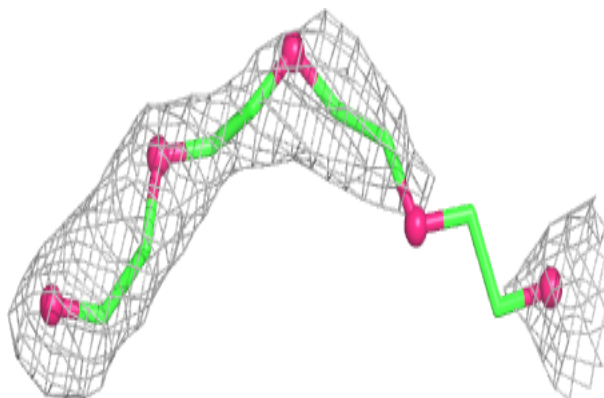
Electron density around C8E A 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
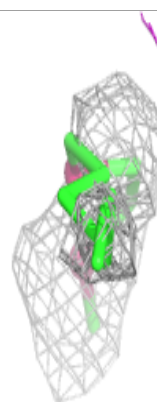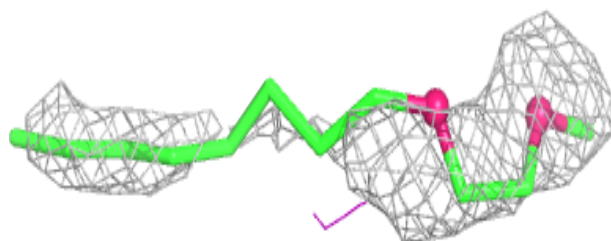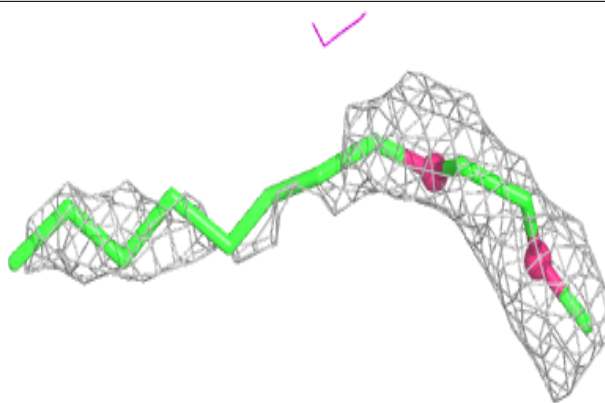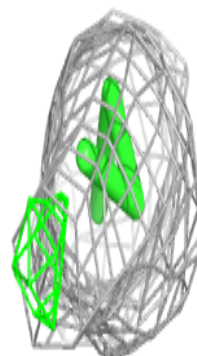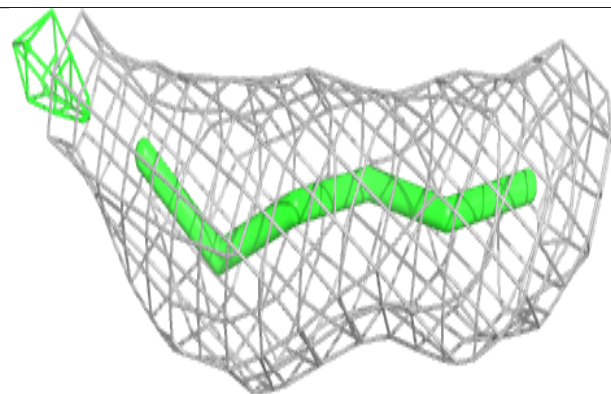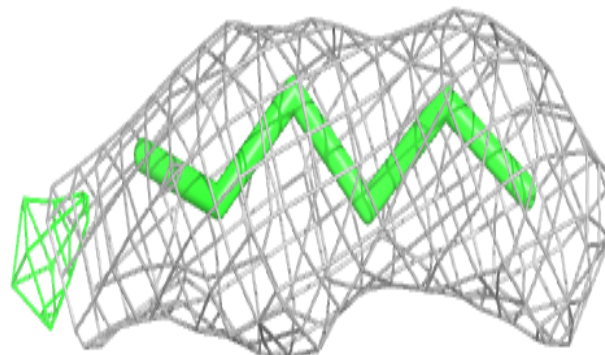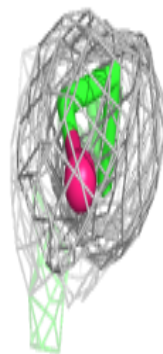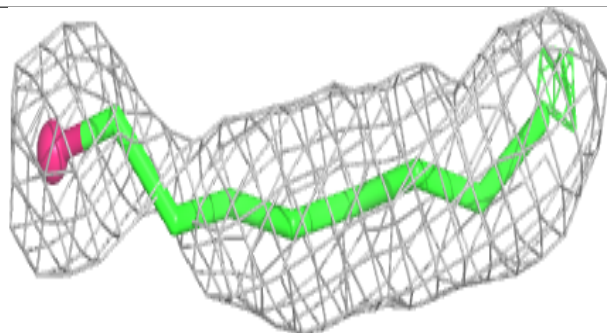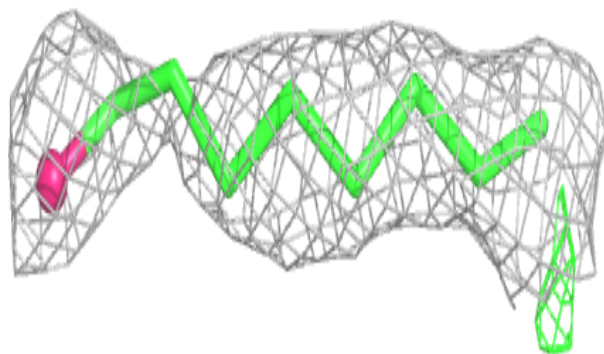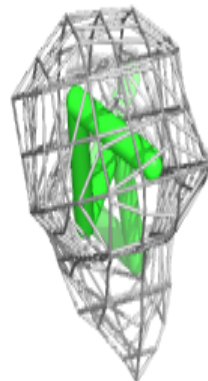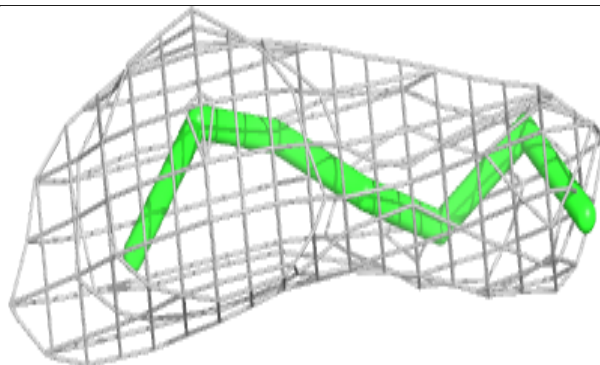and green (positive)
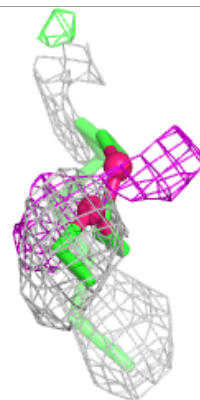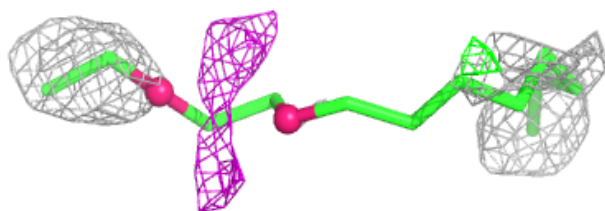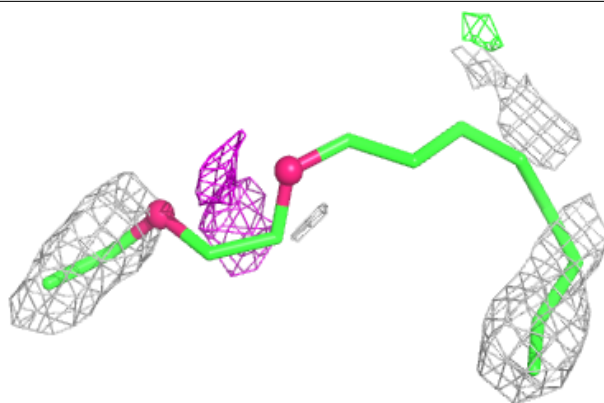
Electron density around C8E A 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
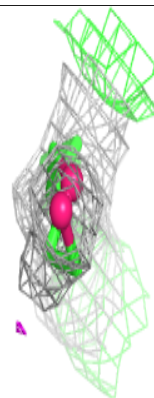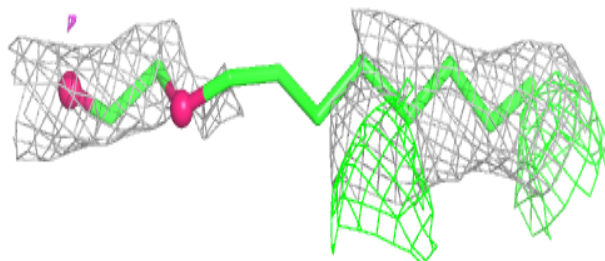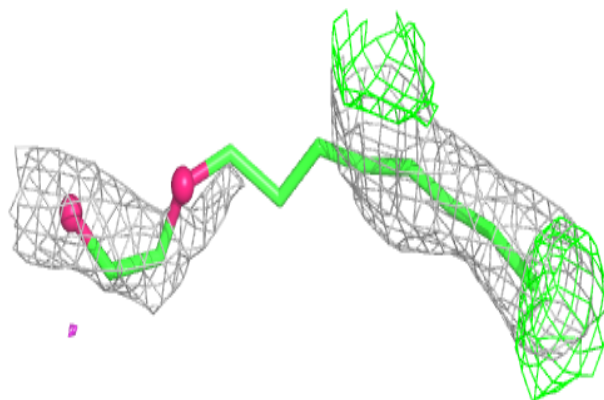
Electron density around C8E A 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
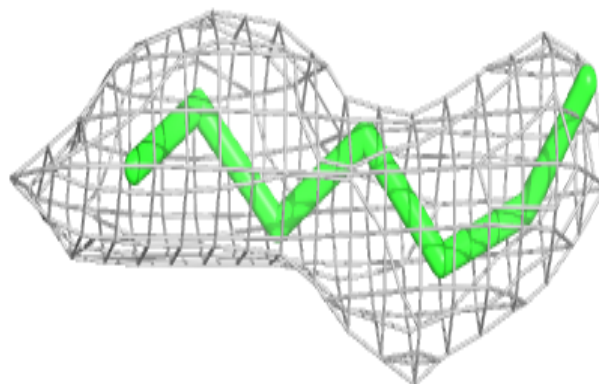and green (positive)
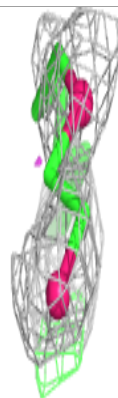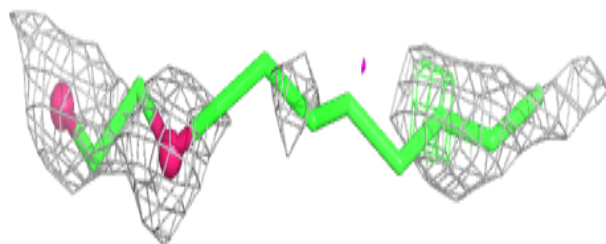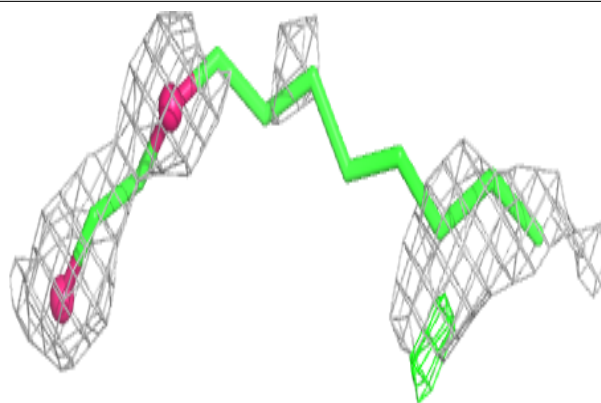
Electron density around C8E A 395:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
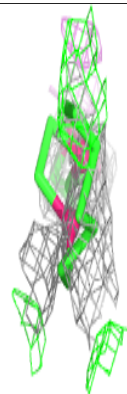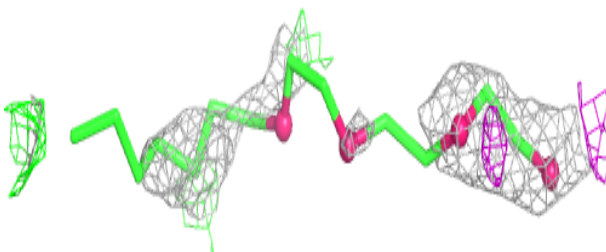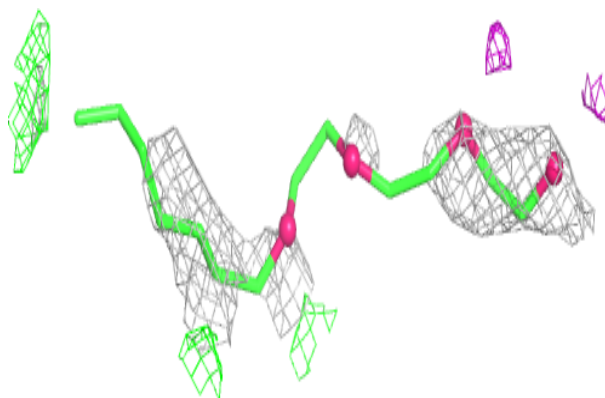
Electron density around C8E B 399:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
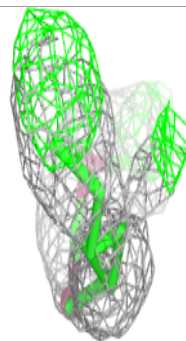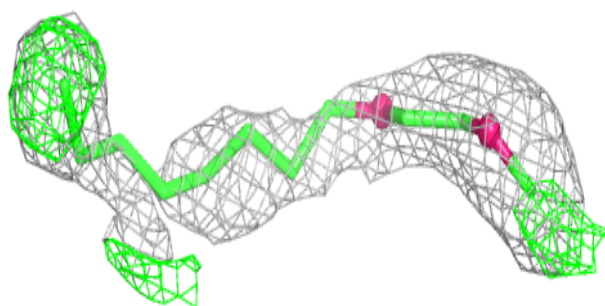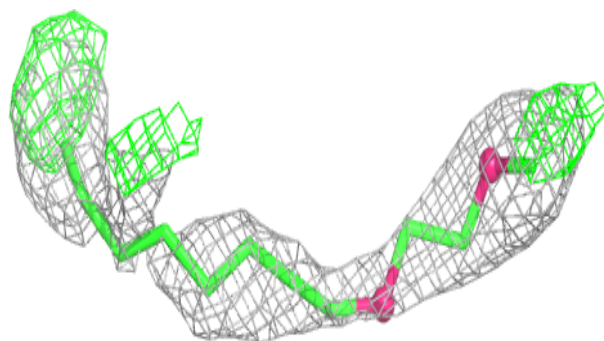
Electron density around C8E A 399:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
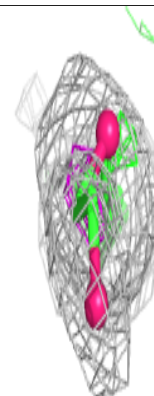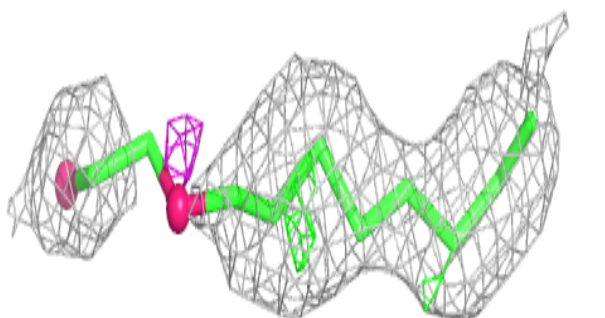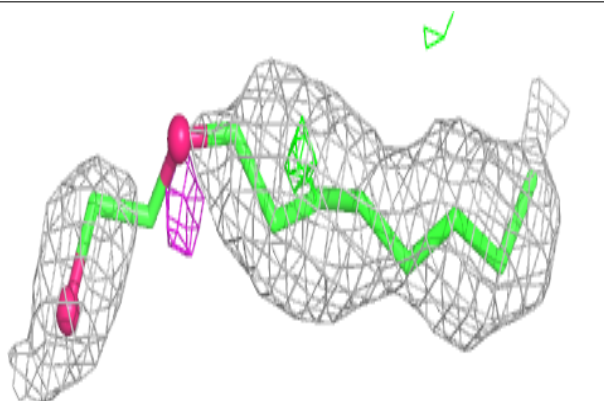
Electron density around C8E B 391:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
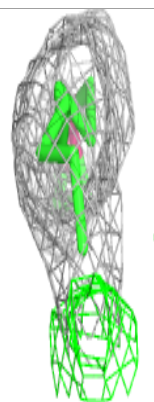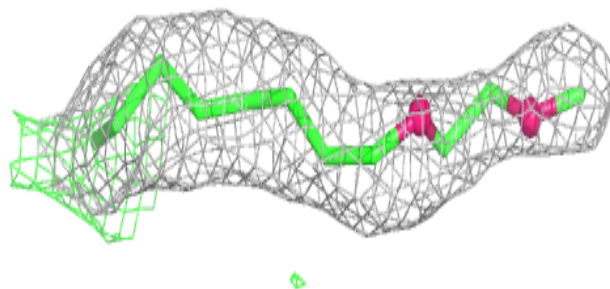and green (positive)
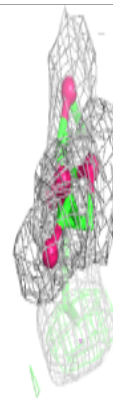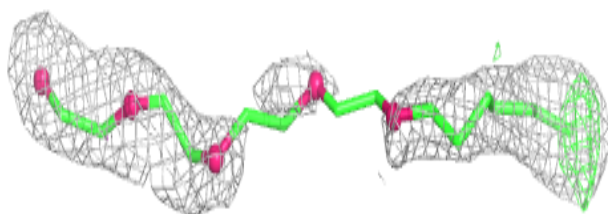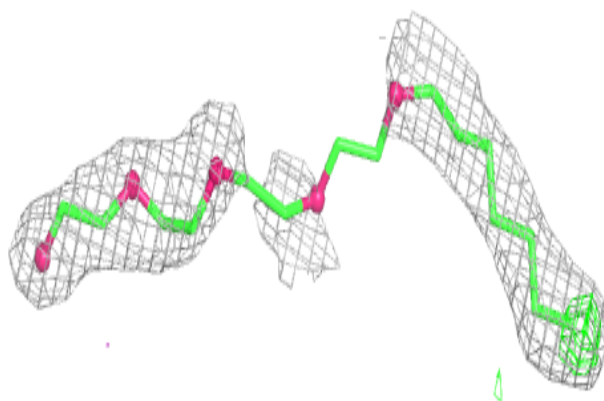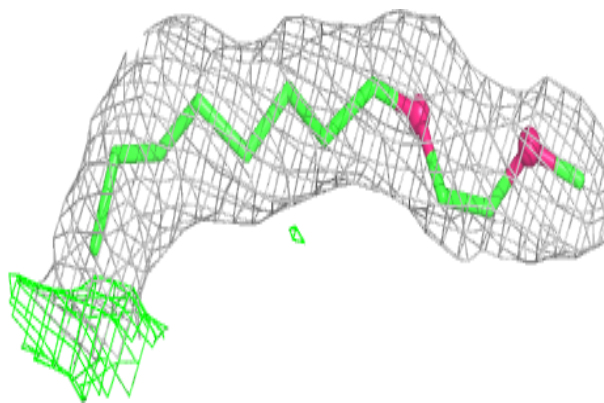

Electron density around C8E B 396:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
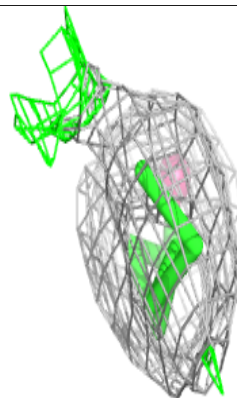and green (positive)
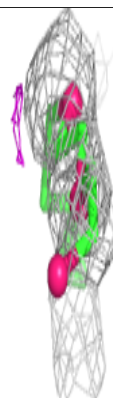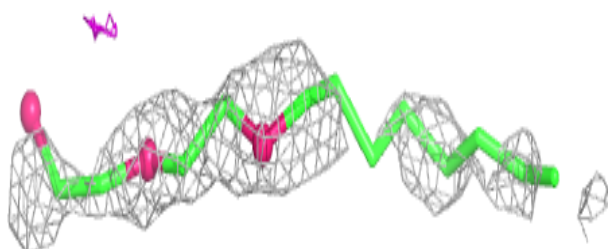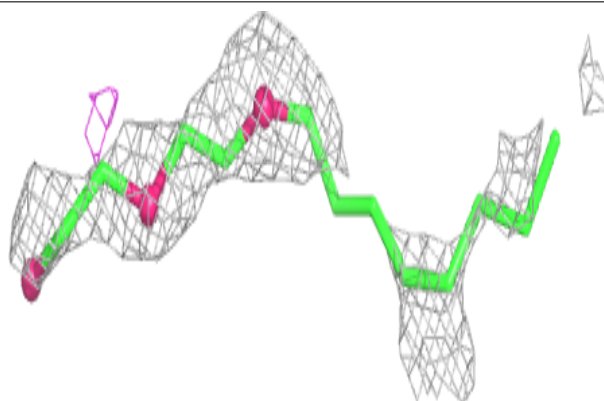
Electron density around C8E A 398:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
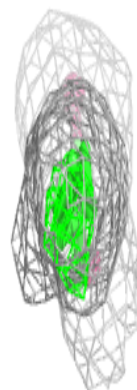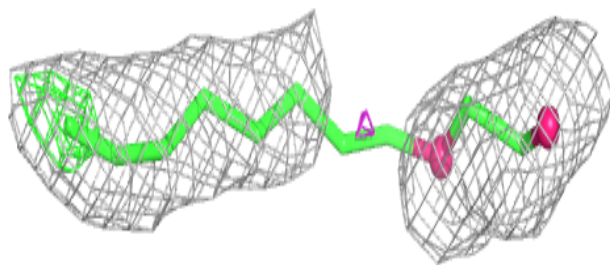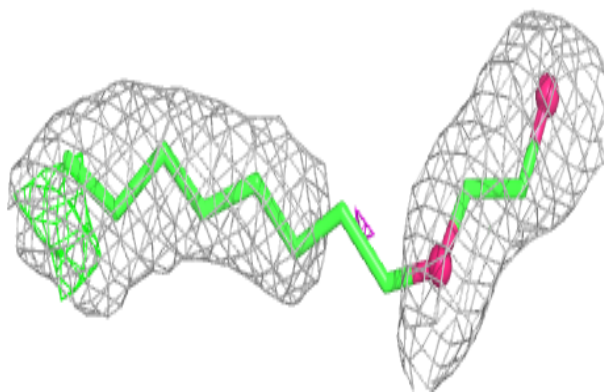
Electron density around C8E B 394:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
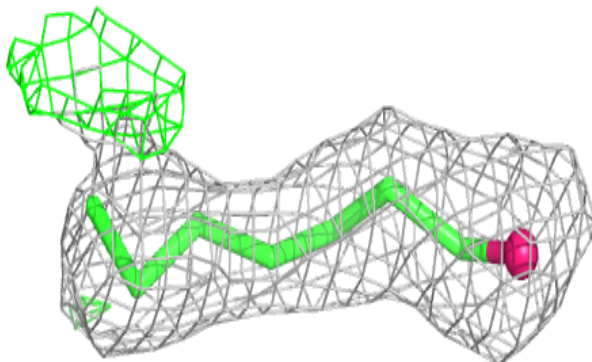mF_o-DF_c (at 3 rmsd) in purple (negative)
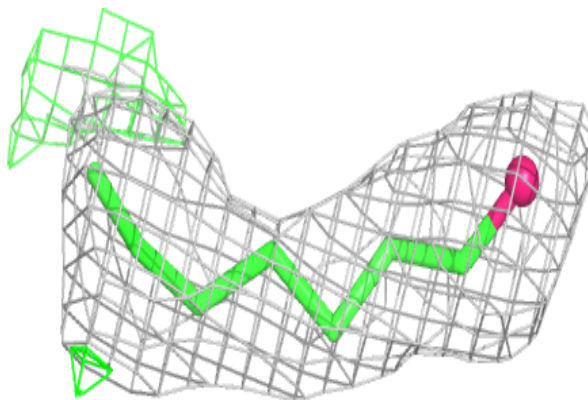and green (positive)
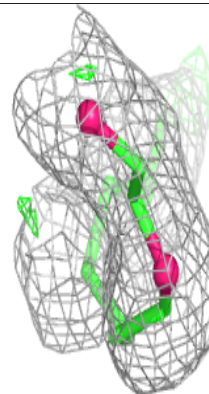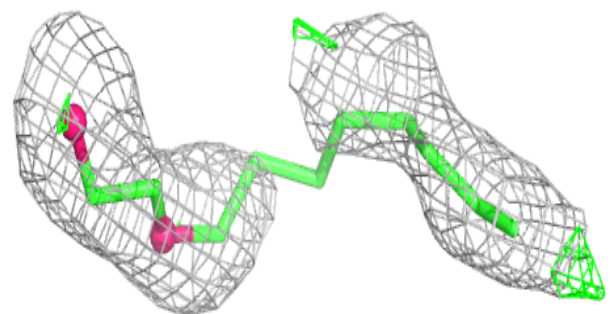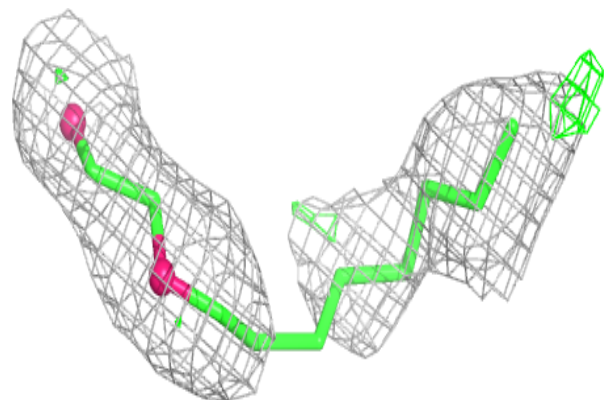
Electron density around C8E A 393:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
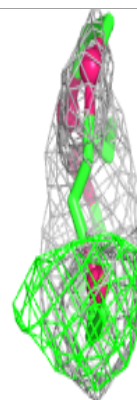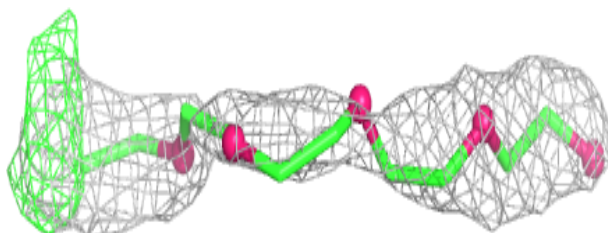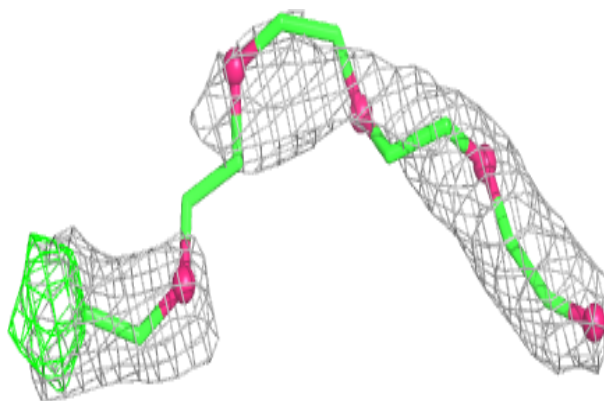
Electron density around C8E B 397:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
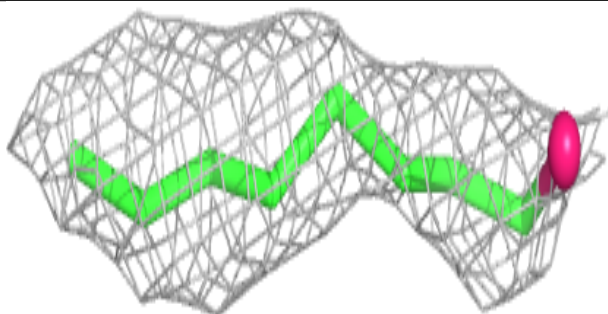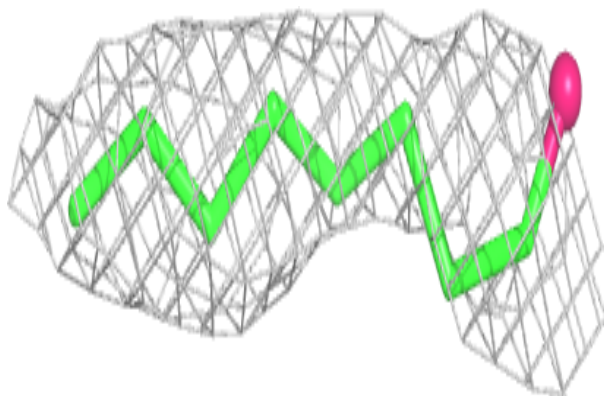
Electron density around C8E B 395:
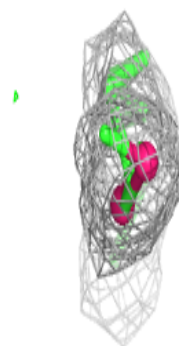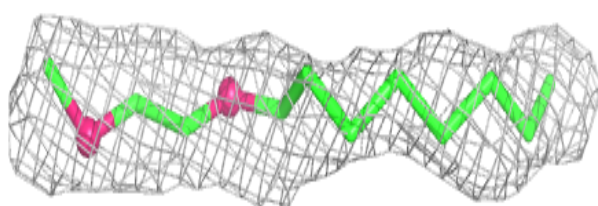
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
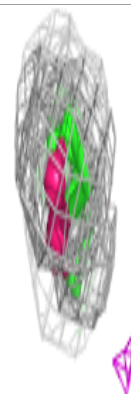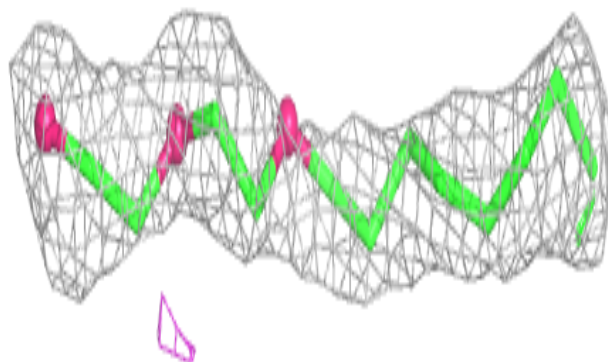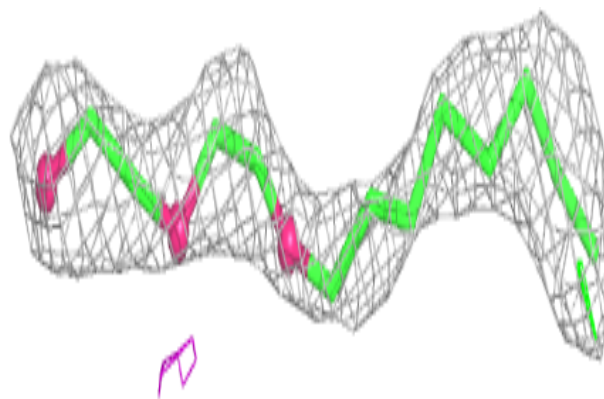
Electron density around C8E B 392:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
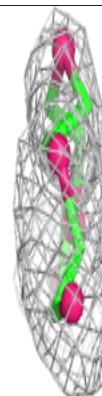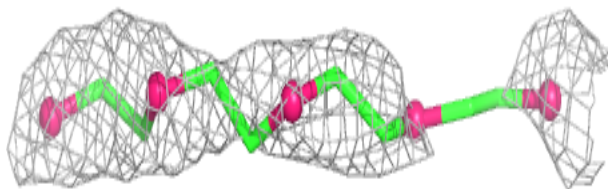
Electron density around C8E B 400:

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

Electron density around C8E A 396:

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

Electron density around C8E A 397:

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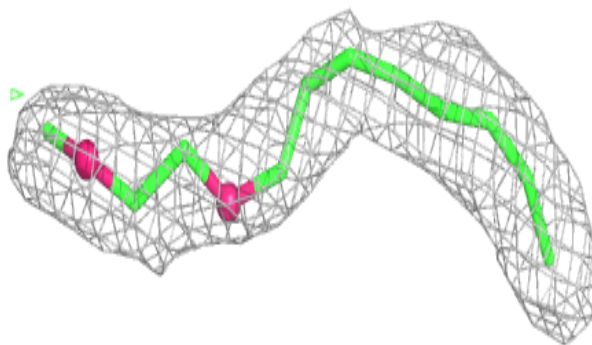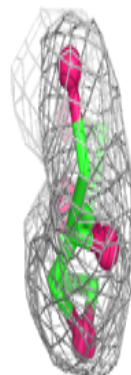and green (positive)

Electron density around C8E B 398:

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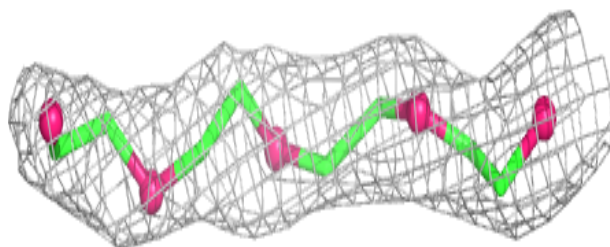and green (positive)

Electron density around C8E A 394:

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 393:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
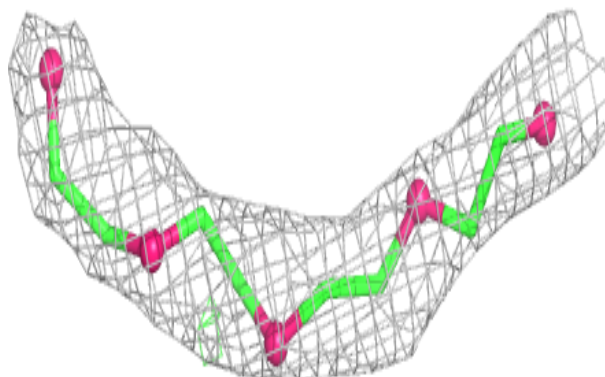and green (positive)

Electron density around C8E A 392:

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 391:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.