Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 05:35 am BST

PDB ID	:	2X4M
Title	:	Yersinia Pestis Plasminogen Activator Pla
Authors	:	Eren, E.; Murphy, M.; Goguen, J.; van den Berg, B.
Deposited on	:	2010-02-05
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

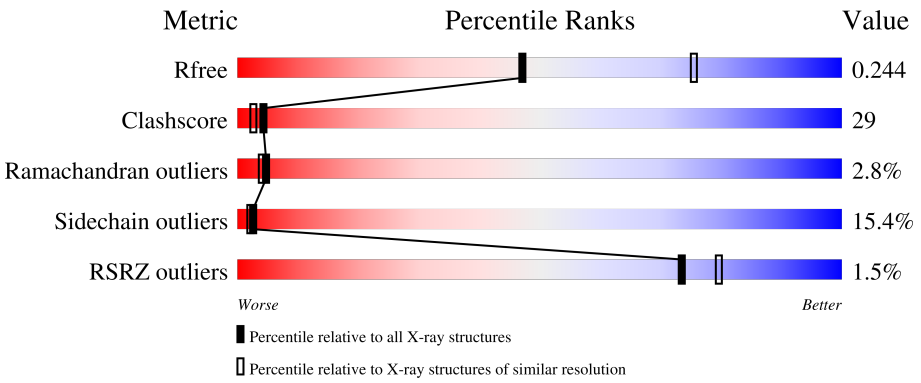
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	298	49% 41% 7% • •
1	B	298	4% 52% 34% 9% •
1	C	298	2% 50% 37% 11% •
1	D	298	51% 38% 9% • •

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	SO4	B	1302	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9482 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 COAGULASE/FIBRINOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2305	1450	393	456	6	0	0	0
			Total	C	N	O	S			
1	B	286	2242	1409	384	443	6	0	0	0
			Total	C	N	O	S			
1	C	291	2262	1419	389	448	6	0	0	0
			Total	C	N	O	S			
1	D	293	2305	1450	393	456	6	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	ASP	engineered mutation	UNP P17811
B	86	ALA	ASP	engineered mutation	UNP P17811
C	86	ALA	ASP	engineered mutation	UNP P17811
D	86	ALA	ASP	engineered mutation	UNP P17811
A	293	GLY	-	expression tag	UNP P17811
A	294	GLY	-	expression tag	UNP P17811
A	295	GLY	-	expression tag	UNP P17811
A	296	GLY	-	expression tag	UNP P17811
A	297	GLY	-	expression tag	UNP P17811
A	298	GLY	-	expression tag	UNP P17811
B	293	GLY	-	expression tag	UNP P17811
B	294	GLY	-	expression tag	UNP P17811
B	295	GLY	-	expression tag	UNP P17811
B	296	GLY	-	expression tag	UNP P17811
B	297	GLY	-	expression tag	UNP P17811
B	298	GLY	-	expression tag	UNP P17811
C	293	GLY	-	expression tag	UNP P17811
C	294	GLY	-	expression tag	UNP P17811
C	295	GLY	-	expression tag	UNP P17811
C	296	GLY	-	expression tag	UNP P17811
C	297	GLY	-	expression tag	UNP P17811

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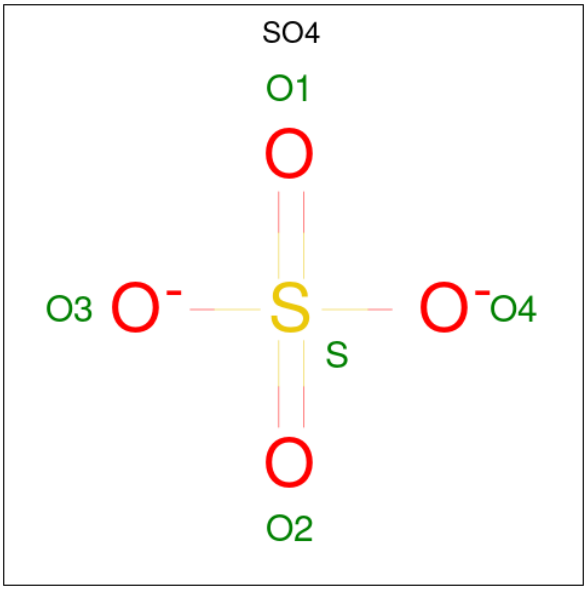
Chain	Residue	Modelled	Actual	Comment	Reference
C	298	GLY	-	expression tag	UNP P17811
D	293	GLY	-	expression tag	UNP P17811
D	294	GLY	-	expression tag	UNP P17811
D	295	GLY	-	expression tag	UNP P17811
D	296	GLY	-	expression tag	UNP P17811
D	297	GLY	-	expression tag	UNP P17811
D	298	GLY	-	expression tag	UNP P17811

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0

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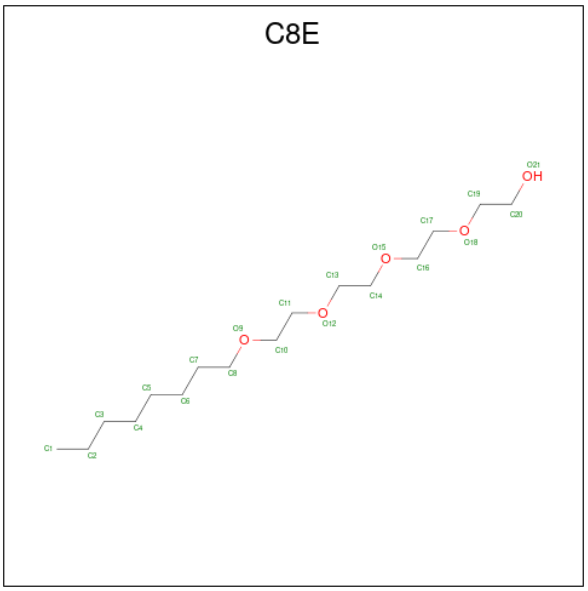
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 10 1	0	0
3	A	1	Total C O 9 8 1	0	0
3	A	1	Total C O 9 8 1	0	0
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C 8 8	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C O 8 7 1	0	0
3	B	1	Total C O 11 9 2	0	0
3	C	1	Total C O 11 10 1	0	0
3	C	1	Total C O 9 8 1	0	0
3	C	1	Total C O 9 8 1	0	0
3	D	1	Total C O 12 10 2	0	0
3	D	1	Total C O 9 8 1	0	0
3	D	1	Total C O 9 8 1	0	0

- Molecule 4 is water.

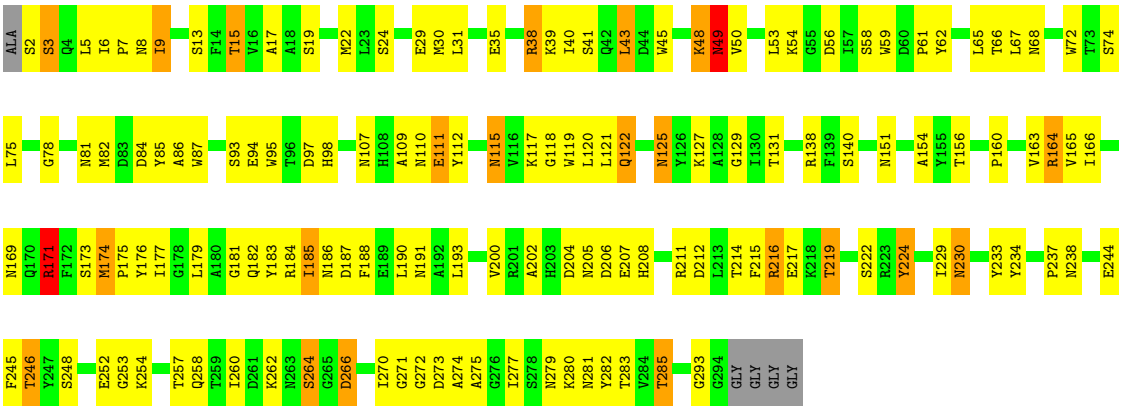
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	33	33	33	0	0
			Total	O		
4	B	30	30	30	0	0
			Total	O		
4	C	30	30	30	0	0
			Total	O		
4	D	27	27	27	0	0

3 Residue-property plots (i)

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.

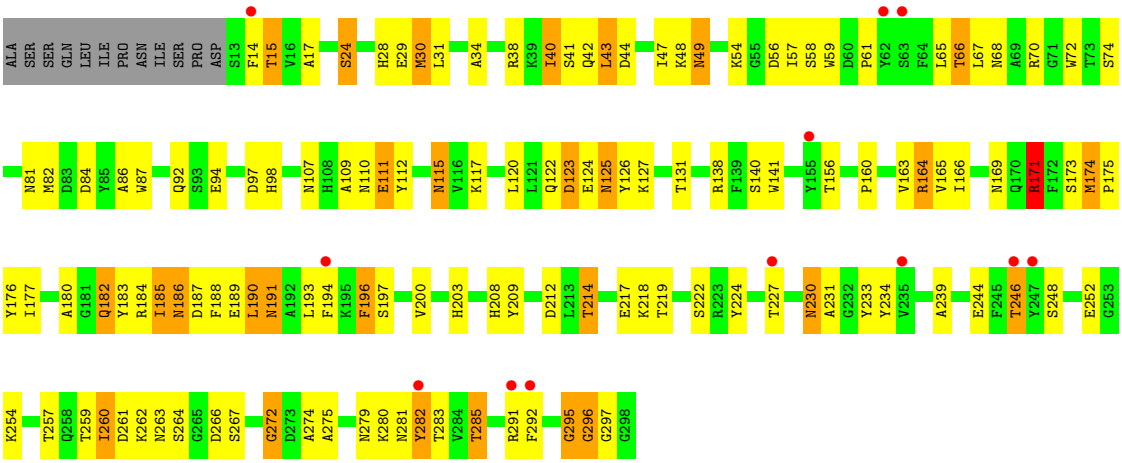
• Molecule 1: COAGULASE/FIBRINOLYSIN

Chain A:



• Molecule 1: COAGULASE/FIBRINOLYSIN

Chain B:



• Molecule 1: COAGULASE/FIBRINOLYSIN

Chain C:

ALA SER S3 Q4 L5 I6 P7 N8 I9 S10 P11 D12 S13 F14 T15 V16 A17 M22 L23 S24 H28 E29 M30 L31 Y32 D33 A34 E35 T36 G37 R38 K39 I40 S41 Q42 L43 D44 I47 K48 N49 V50 A51 I52 L53 K54 G55 D56 I57 S58 W59 D60 P61 Y62 L65 T66 L67

N68 A69 R70 G71 W72 T73 S74 G78 S79 G80 N81 M82 D83 D84 Y85 A86 N89 E90 N91 Q92 S93 E94 D97 H98 N107 H108 A109 N110 E111 Y112 N115 V116 K117 G118 W119 L120 L121 E124 N125 Y126 K127 A128 G129 I130 T131 Q135 S140 W141 S147 T156

G157 P160 V163 R164 V165 I166 N169 Q170 R171 F172 S173 M174 P175 Y176 I177 G178 L179 Q182 D187 F188 N191 A192 L193 F196 S197 V200 R201 D206 E207 H208 Y209 M210 R211 D212 L213 T214 F215 K218 T219 S222 R223 Y224 T227 V228 I229 N230 V235

E244 F245 T246 Y247 S248 E252 G253 K254 T257 I260 D266 S267 V268 D273 A274 A275 N279 K280 N281 Y282 T285 G293 GLY GLY GLY GLY GLY

- Molecule 1: COAGULASE/FIBRINOLYSIN

Chain D: 51% 38% 9%

ALA S2 S3 Q4 L5 I6 P7 N8 I9 S10 P11 D12 T15 V16 A17 M22 L23 S24 H28 E29 M30 L31 Y32 D33 T36 G37 R38 S41 Q42 L43 D44 I47 K48 N49 V50 A51 D56 I57 S58 W59 D60 P61 T66 L67 N68 A69 R70 S74 G78

N81 M82 D83 D84 Y85 A86 W87 M88 N89 Q92 W95 T96 D97 H98 P102 N107 H108 A109 N110 E111 Y112 N115 V116 K117 G118 W119 L120 D123 E124 N125 Y126 T131 R138 F139 S140 S147 Y148 S149 N152 T156 G157 N158 F159 P160 K161 G162 V163 R164 V165

I166 N169 Q170 R171 F172 S173 M174 P175 Y176 A180 G181 Q182 Y183 R184 I185 N186 D187 F188 E189 L190 N191 A192 L193 F194 K195 F196 S197 D198 W199 V200 R201 A202 H203 D204 H208 R211 D212 L213 T214 E217 K218 T219 S220 G221 S222 R223 Y224 T227 N230 E244 F245 T246

Y247 S248 D251 E252 G253 K254 T257 Q258 T259 I260 D261 K262 N263 S264 S267 A274 A275 G276 I277 S278 N279 K280 N281 Y282 T283 Y284 T285 F292 G293 G294 GLY GLY GLY GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.91Å 127.82Å 107.17Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	19.93 – 2.55 35.72 – 2.54	Depositor EDS
% Data completeness (in resolution range)	92.6 (19.93-2.55) 91.6 (35.72-2.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.246 0.188 , 0.244	Depositor DCC
R_{free} test set	2004 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.288 for h,-k,-l	Xtriage
Reported twinning fraction	0.321 for h,-k,-l	Depositor
Outliers	1 of 59361 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9482	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.45	0/2366	0.65	2/3208 (0.1%)
1	B	0.45	0/2301	0.65	2/3116 (0.1%)
1	C	0.44	0/2321	0.80	3/3141 (0.1%)
1	D	0.46	0/2366	0.65	2/3208 (0.1%)
All	All	0.45	0/9354	0.69	9/12673 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	171	ARG	NE-CZ-NH1	-18.99	110.81	120.30
1	C	171	ARG	NE-CZ-NH2	18.19	129.40	120.30
1	C	171	ARG	CD-NE-CZ	8.99	136.19	123.60
1	D	171	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	171	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	171	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	171	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	171	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	171	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2305	0	2141	129	1
1	B	2242	0	2077	131	2
1	C	2262	0	2070	135	2
1	D	2305	0	2141	139	1
2	A	25	0	0	2	0
2	B	25	0	0	2	0
2	C	30	0	0	3	0
2	D	35	0	0	2	0
3	A	47	0	85	7	0
3	B	27	0	43	3	0
3	C	29	0	53	0	0
3	D	30	0	55	0	0
4	A	33	0	0	4	0
4	B	30	0	0	5	0
4	C	30	0	0	2	0
4	D	27	0	0	2	0
All	All	9482	0	8665	526	3

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 29.

All (526) 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:C:38:ARG:HG3	1:C:38:ARG:HH11	1.01	1.17
1:C:13:SER:HB3	1:C:59:TRP:HZ3	1.08	1.09
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.11	1.08
1:C:13:SER:HB3	1:C:59:TRP:CZ3	1.93	1.03
1:D:117:LYS:HG3	1:D:131:THR:HG22	1.40	1.03
1:B:117:LYS:HG3	1:B:131:THR:HG22	1.41	1.02
1:B:234:TYR:HD2	4:B:2023:HOH:O	1.42	1.02
1:D:12:ASP:HB2	1:D:59:TRP:CZ3	1.95	1.01
1:A:117:LYS:HG3	1:A:131:THR:HG22	1.41	1.00
1:C:117:LYS:HG3	1:C:131:THR:HG22	1.45	0.98
1:B:164:ARG:HG3	1:B:164:ARG:HH11	1.27	0.98
1:D:12:ASP:HB2	1:D:59:TRP:HZ3	1.31	0.95
1:D:36:THR:HG22	1:D:38:ARG:H	1.32	0.94
1:C:57:ILE:HG22	1:C:69:ALA:HB3	1.50	0.93
1:A:13:SER:HA	1:A:293:GLY:HA2	1.51	0.92
1:C:248:SER:HB2	1:C:281:ASN:HB2	1.54	0.90
1:D:89:ASN:HB3	1:D:92:GLN:HB3	1.53	0.90
1:C:50:VAL:HG22	1:C:78:GLY:HA3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:HA3	3:A:1302:C8E:H81	1.56	0.88
1:C:267:SER:O	1:C:268:VAL:HG23	1.74	0.87
1:D:248:SER:HB2	1:D:281:ASN:HB2	1.56	0.87
1:A:164:ARG:HG2	1:A:164:ARG:NH1	1.88	0.86
1:D:31:LEU:HB3	1:D:41:SER:HB3	1.58	0.86
1:B:248:SER:HB2	1:B:281:ASN:HB2	1.57	0.85
1:B:164:ARG:HH11	1:B:164:ARG:CG	1.89	0.85
1:C:38:ARG:HG3	1:C:38:ARG:NH1	1.81	0.85
1:B:24:SER:HB3	1:B:282:TYR:HD2	1.40	0.84
1:D:217:GLU:HB3	1:D:277:ILE:HD11	1.61	0.81
1:A:248:SER:HB2	1:A:281:ASN:HB2	1.62	0.81
1:D:263:ASN:C	1:D:263:ASN:HD22	1.84	0.80
1:B:24:SER:HB3	1:B:282:TYR:CD2	2.17	0.80
1:C:89:ASN:HD22	1:C:90:GLU:N	1.81	0.79
1:C:12:ASP:O	1:C:13:SER:HB2	1.81	0.78
1:C:147:SER:OG	1:D:6:ILE:HD11	1.83	0.78
1:B:59:TRP:HD1	1:B:67:LEU:HD12	1.49	0.78
1:A:204:ASP:OD1	1:A:217:GLU:HB2	1.83	0.78
1:A:164:ARG:HH11	1:A:164:ARG:CG	1.93	0.77
1:A:38:ARG:CZ	1:A:39:LYS:H	1.97	0.77
1:A:15:THR:HG22	1:A:58:SER:HB3	1.65	0.77
1:C:13:SER:CB	1:C:59:TRP:HZ3	1.95	0.76
1:B:56:ASP:OD2	1:B:57:ILE:N	2.19	0.76
1:B:234:TYR:CD2	4:B:2023:HOH:O	2.26	0.75
1:D:66:THR:HG23	1:D:119:TRP:HE1	1.51	0.74
1:A:200:VAL:HB	1:A:222:SER:OG	1.88	0.74
1:D:36:THR:HG22	1:D:38:ARG:N	2.03	0.73
1:A:54:LYS:CG	1:A:72:TRP:HB3	2.19	0.72
1:D:214:THR:HG23	1:D:260:ILE:HG23	1.71	0.72
1:B:54:LYS:NZ	1:B:54:LYS:HB3	2.02	0.72
1:D:185:ILE:HG23	1:D:185:ILE:O	1.90	0.71
1:C:38:ARG:HH11	1:C:38:ARG:CG	1.92	0.71
1:A:13:SER:HA	1:A:293:GLY:CA	2.20	0.70
1:D:92:GLN:HE22	1:D:152:ASN:HD21	1.39	0.70
1:C:227:THR:HG22	1:C:247:TYR:HB3	1.74	0.69
1:A:6:ILE:HD12	1:A:186:ASN:HA	1.74	0.69
1:B:194:PHE:CE2	1:B:196:PHE:CD1	2.80	0.69
1:B:190:LEU:HG	1:B:191:ASN:N	2.07	0.69
1:D:12:ASP:CB	1:D:59:TRP:CZ3	2.74	0.69
1:A:7:PRO:HG3	1:A:234:TYR:CD1	2.28	0.69
1:B:239:ALA:N	4:B:2023:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HG3	1:A:72:TRP:HB3	1.75	0.68
1:D:148:TYR:CZ	1:D:157:GLY:HA3	2.28	0.68
1:C:12:ASP:O	1:C:13:SER:CB	2.42	0.68
1:C:57:ILE:CG2	1:C:69:ALA:HB3	2.23	0.67
1:C:9:ILE:H	1:C:14:PHE:HE1	1.43	0.67
1:B:166:ILE:HD12	1:B:208:HIS:CE1	2.29	0.67
1:D:117:LYS:HG3	1:D:131:THR:CG2	2.22	0.67
1:C:91:ASN:OD1	1:C:92:GLN:N	2.28	0.67
1:B:38:ARG:NH2	1:B:87:TRP:O	2.28	0.67
1:C:91:ASN:O	1:C:92:GLN:HB3	1.94	0.67
1:C:118:GLY:O	1:C:129:GLY:HA3	1.94	0.67
1:C:191:ASN:HD22	1:C:230:ASN:ND2	1.92	0.67
1:D:12:ASP:HB2	1:D:59:TRP:CH2	2.30	0.66
1:B:176:TYR:O	1:B:177:ILE:HD13	1.95	0.66
1:D:66:THR:CG2	1:D:119:TRP:HE1	2.09	0.66
1:C:191:ASN:HD22	1:C:230:ASN:HD21	1.43	0.66
1:C:38:ARG:HE	1:C:90:GLU:HG3	1.60	0.65
1:C:147:SER:HB2	1:C:157:GLY:O	1.96	0.65
1:D:59:TRP:O	1:D:61:PRO:HD3	1.96	0.65
1:D:92:GLN:HE22	1:D:152:ASN:ND2	1.94	0.65
1:A:160:PRO:HB2	1:A:163:VAL:HG21	1.79	0.65
1:B:212:ASP:C	1:B:262:LYS:HG2	2.17	0.65
1:B:59:TRP:CH2	1:B:296:GLY:O	2.50	0.65
1:B:40:ILE:O	1:B:86:ALA:HA	1.97	0.64
1:C:160:PRO:O	1:C:163:VAL:HG22	1.98	0.64
1:B:212:ASP:O	1:B:262:LYS:HG2	1.98	0.64
1:B:126:TYR:CZ	1:B:183:TYR:CE1	2.85	0.64
1:D:147:SER:HB3	1:D:158:ASN:HD22	1.63	0.63
1:B:61:PRO:HG2	1:B:65:LEU:HD23	1.80	0.63
1:C:219:THR:HG21	1:C:253:GLY:HA3	1.81	0.63
1:C:117:LYS:HG3	1:C:131:THR:CG2	2.26	0.62
1:D:160:PRO:HB2	1:D:163:VAL:HG21	1.81	0.62
1:A:175:PRO:HB2	3:A:1303:C8E:H61	1.82	0.62
1:C:191:ASN:ND2	1:C:230:ASN:HD21	1.98	0.62
1:A:6:ILE:CD1	1:A:186:ASN:HA	2.30	0.62
1:B:257:THR:HG22	1:B:275:ALA:HB2	1.82	0.62
1:D:17:ALA:HB3	1:D:56:ASP:HB3	1.81	0.62
1:D:36:THR:CG2	1:D:38:ARG:HB2	2.29	0.62
1:B:54:LYS:HD3	1:B:285:THR:HG21	1.82	0.62
1:B:182:GLN:HG2	1:B:183:TYR:N	2.15	0.62
1:A:15:THR:CG2	1:A:58:SER:HB3	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HD12	1:A:184:ARG:NH1	2.16	0.61
1:B:200:VAL:HB	1:B:222:SER:OG	2.00	0.61
1:C:15:THR:HG22	1:C:58:SER:HB2	1.83	0.61
1:A:230:ASN:C	1:A:230:ASN:HD22	2.04	0.61
1:A:117:LYS:HG3	1:A:131:THR:CG2	2.24	0.61
1:A:205:ASN:HD21	1:A:216:ARG:NH2	1.98	0.61
1:B:48:LYS:O	1:B:49:ASN:C	2.39	0.61
1:B:117:LYS:HG3	1:B:131:THR:CG2	2.26	0.61
1:B:126:TYR:CZ	1:B:183:TYR:CD1	2.88	0.61
1:B:180:ALA:C	3:B:1306:C8E:H81	2.21	0.61
1:C:9:ILE:O	1:C:11:PRO:N	2.34	0.60
1:C:43:LEU:N	1:C:43:LEU:CD2	2.64	0.60
1:B:92:GLN:HG2	1:B:94:GLU:O	2.02	0.60
1:D:208:HIS:HB3	1:D:211:ARG:HG2	1.83	0.60
1:A:67:LEU:HD23	1:A:67:LEU:N	2.16	0.60
1:C:257:THR:HG22	1:C:275:ALA:HB2	1.82	0.60
1:A:214:THR:HB	1:A:260:ILE:HD13	1.84	0.60
1:A:29:GLU:HB3	1:A:43:LEU:HB2	1.84	0.60
1:D:164:ARG:CG	1:D:164:ARG:HH11	2.14	0.60
1:A:175:PRO:HD3	4:A:2016:HOH:O	2.03	0.59
1:D:200:VAL:HB	1:D:222:SER:HB2	1.84	0.59
1:D:257:THR:HG22	1:D:275:ALA:HB2	1.82	0.59
1:B:54:LYS:HG2	1:B:72:TRP:HB3	1.85	0.59
1:C:89:ASN:HD22	1:C:89:ASN:C	2.06	0.59
1:D:131:THR:CG2	1:D:180:ALA:HB2	2.33	0.59
1:B:188:PHE:CD2	1:B:189:GLU:N	2.71	0.59
1:A:188:PHE:CZ	1:A:190:LEU:HB2	2.37	0.59
1:C:268:VAL:HG12	1:C:268:VAL:O	2.01	0.59
1:A:257:THR:HG22	1:A:275:ALA:HB2	1.85	0.59
1:C:61:PRO:HB2	1:C:62:TYR:CD1	2.39	0.58
1:C:65:LEU:HD12	1:C:117:LYS:O	2.03	0.58
1:B:31:LEU:HG	1:B:40:ILE:HD11	1.84	0.58
1:B:48:LYS:O	1:B:49:ASN:O	2.21	0.58
1:D:28:HIS:HD2	1:D:42:GLN:HE21	1.50	0.58
1:A:119:TRP:CE3	1:A:127:LYS:HG2	2.38	0.58
1:B:111:GLU:HG2	1:B:112:TYR:N	2.18	0.58
1:B:160:PRO:HB2	1:B:163:VAL:CG2	2.34	0.58
1:C:174:MET:CE	1:C:200:VAL:HG22	2.33	0.58
1:D:182:GLN:HG3	1:D:191:ASN:OD1	2.04	0.58
1:D:252:GLU:OE2	1:D:254:LYS:HE2	2.04	0.58
1:C:192:ALA:HA	1:C:228:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:THR:HG21	1:D:38:ARG:NH1	2.19	0.58
1:A:38:ARG:NE	1:A:38:ARG:HA	2.19	0.58
1:B:230:ASN:C	1:B:230:ASN:HD22	2.07	0.58
1:C:4:GLN:O	1:C:6:ILE:N	2.37	0.58
1:C:165:VAL:HG12	1:C:166:ILE:HG12	1.85	0.58
1:D:204:ASP:OD1	1:D:217:GLU:HB2	2.04	0.58
1:A:59:TRP:O	1:A:61:PRO:HD3	2.04	0.57
1:A:206:ASP:HB3	1:A:215:PHE:HB2	1.85	0.57
1:B:185:ILE:HG23	1:B:185:ILE:O	2.04	0.57
1:D:5:LEU:HD23	1:D:5:LEU:C	2.24	0.57
1:C:84:ASP:O	1:C:98:HIS:HA	2.05	0.57
1:C:174:MET:HE3	1:C:200:VAL:HG22	1.84	0.57
1:D:176:TYR:CE1	1:D:195:LYS:HG2	2.40	0.57
1:A:122:GLN:HG2	1:A:127:LYS:HG3	1.87	0.57
1:B:86:ALA:HB3	1:B:97:ASP:HB2	1.87	0.57
1:B:98:HIS:CE1	4:B:2005:HOH:O	2.57	0.57
1:D:28:HIS:CD2	1:D:42:GLN:HE21	2.23	0.57
1:D:164:ARG:HH11	1:D:164:ARG:HG2	1.70	0.57
1:B:97:ASP:OD2	2:B:1302:SO4:O2	2.23	0.57
1:A:84:ASP:O	1:A:98:HIS:HA	2.04	0.56
1:C:22:MET:HE2	1:C:49:ASN:HA	1.87	0.56
1:D:263:ASN:C	1:D:263:ASN:ND2	2.56	0.56
1:C:38:ARG:HH21	1:C:90:GLU:HG2	1.70	0.56
1:C:9:ILE:N	1:C:14:PHE:HE1	2.04	0.56
1:C:28:HIS:HD2	1:C:42:GLN:HE21	1.51	0.56
1:D:174:MET:CE	1:D:200:VAL:HG22	2.35	0.56
1:A:19:SER:O	1:A:53:LEU:HD12	2.06	0.56
1:A:119:TRP:HB2	1:A:122:GLN:OE1	2.06	0.56
1:B:182:GLN:HG2	1:B:183:TYR:H	1.71	0.56
1:D:131:THR:HG21	1:D:193:LEU:HD11	1.88	0.56
1:A:179:LEU:O	1:A:193:LEU:HD12	2.05	0.56
1:B:54:LYS:HB3	1:B:54:LYS:HZ2	1.71	0.55
1:C:212:ASP:O	1:C:213:LEU:HD23	2.06	0.55
1:B:56:ASP:O	1:B:57:ILE:HG13	2.06	0.55
1:D:230:ASN:HD22	1:D:230:ASN:C	2.09	0.55
1:C:50:VAL:CG2	1:C:78:GLY:HA3	2.33	0.55
1:D:6:ILE:HG22	1:D:7:PRO:HD2	1.86	0.55
1:D:161:LYS:HD3	2:D:1296:SO4:O1	2.07	0.55
1:D:174:MET:HE1	1:D:197:SER:HB3	1.88	0.55
1:B:165:VAL:HG12	1:B:166:ILE:HG12	1.87	0.55
1:B:188:PHE:CD2	1:B:188:PHE:C	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ASN:HB2	1:D:115:ASN:OD1	2.06	0.55
1:B:160:PRO:HB2	1:B:163:VAL:HG21	1.89	0.55
1:A:49:ASN:CG	1:A:49:ASN:O	2.44	0.55
1:A:257:THR:CG2	1:A:275:ALA:HB2	2.35	0.55
1:B:30:MET:SD	1:B:42:GLN:HG3	2.47	0.55
1:C:59:TRP:NE1	1:C:61:PRO:HG3	2.21	0.55
1:C:187:ASP:O	1:C:188:PHE:CB	2.53	0.55
1:A:31:LEU:HB3	1:A:41:SER:HB3	1.88	0.54
1:A:160:PRO:HB2	1:A:163:VAL:CG2	2.38	0.54
1:B:214:THR:HG22	1:B:260:ILE:HG23	1.90	0.54
1:C:207:GLU:HG3	1:C:214:THR:HG23	1.90	0.54
1:A:279:ASN:CG	1:A:280:LYS:N	2.61	0.54
1:C:126:TYR:OH	2:C:1295:SO4:O1	2.18	0.54
1:A:177:ILE:HD11	3:A:1303:C8E:C5	2.36	0.54
1:B:28:HIS:HD2	1:B:44:ASP:OD2	1.90	0.54
1:B:61:PRO:O	1:B:297:GLY:HA3	2.07	0.54
1:D:160:PRO:HB2	1:D:163:VAL:CG2	2.38	0.54
1:D:257:THR:CG2	1:D:275:ALA:HB2	2.37	0.54
1:B:125:ASN:O	1:B:126:TYR:CD1	2.60	0.54
1:C:8:ASN:N	1:C:9:ILE:CA	2.70	0.54
1:C:257:THR:CG2	1:C:275:ALA:HB2	2.38	0.54
1:A:174:MET:CE	1:A:200:VAL:HG22	2.37	0.54
1:A:38:ARG:HA	1:A:38:ARG:HE	1.72	0.54
1:B:164:ARG:HG3	1:B:164:ARG:NH1	2.07	0.54
1:A:6:ILE:HD13	1:A:6:ILE:N	2.22	0.54
1:A:54:LYS:HE2	1:A:244:GLU:OE2	2.07	0.54
1:C:156:THR:CG2	1:D:9:ILE:HG12	2.37	0.54
1:C:48:LYS:HE3	1:C:80:GLY:O	2.08	0.53
1:B:59:TRP:CD1	1:B:67:LEU:HD12	2.38	0.53
1:B:279:ASN:CG	1:B:280:LYS:N	2.61	0.53
1:C:7:PRO:CA	1:C:59:TRP:HH2	2.21	0.53
1:D:279:ASN:CG	1:D:280:LYS:N	2.60	0.53
1:B:257:THR:CG2	1:B:275:ALA:HB2	2.37	0.53
1:D:56:ASP:O	1:D:57:ILE:HG13	2.09	0.53
1:A:94:GLU:CD	1:A:94:GLU:H	2.12	0.53
1:C:127:LYS:HE3	1:C:182:GLN:HE21	1.73	0.53
1:D:23:LEU:HG	1:D:47:ILE:HD11	1.90	0.53
1:B:212:ASP:HB3	1:B:262:LYS:HB2	1.90	0.53
1:C:38:ARG:NE	1:C:90:GLU:HG3	2.23	0.53
1:C:91:ASN:O	1:C:92:GLN:CB	2.57	0.53
1:D:84:ASP:O	1:D:98:HIS:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:HG3	1:C:35:GLU:CG	2.38	0.53
1:C:86:ALA:HB3	1:C:97:ASP:HB2	1.91	0.53
1:D:102:PRO:HD2	4:D:2009:HOH:O	2.09	0.53
1:D:123:ASP:OD2	1:D:126:TYR:HB2	2.08	0.53
1:D:292:PHE:O	1:D:294:GLY:N	2.40	0.53
1:D:12:ASP:CB	1:D:59:TRP:HZ3	2.11	0.53
1:B:84:ASP:O	1:B:98:HIS:HA	2.09	0.52
1:C:111:GLU:HG2	1:C:112:TYR:N	2.25	0.52
1:D:198:ASP:OD1	1:D:223:ARG:NH2	2.41	0.52
1:C:70:ARG:NH2	2:C:1294:SO4:O4	2.42	0.52
1:D:246:THR:O	1:D:282:TYR:HA	2.10	0.52
1:A:35:GLU:HG3	1:C:35:GLU:HB3	1.92	0.52
1:C:279:ASN:CG	1:C:280:LYS:N	2.63	0.52
1:A:2:SER:O	1:A:3:SER:HB2	2.10	0.52
1:C:85:TYR:CE1	1:C:98:HIS:CD2	2.98	0.52
1:D:223:ARG:HG3	1:D:251:ASP:OD2	2.10	0.52
1:D:260:ILE:HG13	1:D:262:LYS:HG2	1.92	0.52
1:A:118:GLY:O	1:A:129:GLY:HA3	2.10	0.52
1:A:244:GLU:HB3	1:A:285:THR:HG22	1.92	0.52
2:B:1302:SO4:O3	2:B:1303:SO4:O3	2.27	0.52
1:B:54:LYS:HB3	1:B:54:LYS:HZ3	1.75	0.51
1:A:62:TYR:HD1	1:A:65:LEU:HD23	1.75	0.51
1:D:165:VAL:HG12	1:D:166:ILE:HG12	1.91	0.51
1:D:190:LEU:HD23	1:D:190:LEU:C	2.31	0.51
1:A:191:ASN:O	1:A:229:ILE:HA	2.10	0.51
1:C:59:TRP:CZ2	1:C:61:PRO:HA	2.46	0.51
1:C:22:MET:HG2	1:C:49:ASN:HA	1.92	0.51
1:D:164:ARG:HG2	1:D:164:ARG:NH1	2.25	0.51
1:A:216:ARG:HB2	1:A:258:GLN:HB3	1.93	0.51
1:C:230:ASN:C	1:C:230:ASN:HD22	2.14	0.51
1:B:31:LEU:HD12	1:B:274:ALA:O	2.11	0.51
1:B:164:ARG:HG2	1:B:209:TYR:CD1	2.46	0.51
1:D:111:GLU:HG2	1:D:112:TYR:N	2.26	0.51
1:A:216:ARG:NH2	2:A:1296:SO4:O2	2.43	0.51
1:C:43:LEU:N	1:C:43:LEU:HD23	2.26	0.51
1:C:244:GLU:HB3	1:C:285:THR:HG22	1.91	0.51
1:D:230:ASN:ND2	4:D:2020:HOH:O	2.44	0.51
1:D:279:ASN:CG	1:D:280:LYS:H	2.14	0.51
1:A:22:MET:SD	1:A:49:ASN:ND2	2.84	0.51
1:C:6:ILE:O	1:C:61:PRO:O	2.28	0.51
1:D:148:TYR:OH	1:D:157:GLY:HA3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:CG2	1:C:38:ARG:HB2	2.41	0.50
1:A:279:ASN:CG	1:A:280:LYS:H	2.15	0.50
1:B:38:ARG:NH1	1:B:40:ILE:HG22	2.26	0.50
1:B:188:PHE:HD1	1:B:233:TYR:CZ	2.29	0.50
1:D:198:ASP:OD1	1:D:223:ARG:NE	2.42	0.50
1:A:230:ASN:C	1:A:230:ASN:ND2	2.63	0.50
1:B:54:LYS:HE3	1:B:244:GLU:OE2	2.11	0.50
1:B:65:LEU:HD12	1:B:117:LYS:O	2.11	0.50
1:B:279:ASN:CG	1:B:280:LYS:H	2.15	0.50
1:C:31:LEU:HB3	1:C:41:SER:HB2	1.94	0.50
1:A:87:TRP:CE2	1:A:95:TRP:HB3	2.46	0.50
1:A:219:THR:HG21	1:A:253:GLY:HA3	1.94	0.50
1:D:203:HIS:HA	1:D:217:GLU:O	2.12	0.50
1:B:194:PHE:CE2	1:B:196:PHE:HD1	2.27	0.50
1:B:244:GLU:HB3	1:B:285:THR:HG22	1.92	0.50
1:B:185:ILE:HG22	1:B:188:PHE:HB3	1.92	0.50
1:D:15:THR:HG22	1:D:58:SER:H	1.76	0.50
1:A:22:MET:HG3	1:A:49:ASN:HD22	1.76	0.50
1:A:224:TYR:C	1:A:224:TYR:CD2	2.86	0.49
1:C:174:MET:HE1	1:C:224:TYR:HB3	1.93	0.49
1:D:125:ASN:O	1:D:183:TYR:HA	2.12	0.49
1:A:50:VAL:HG22	1:A:78:GLY:HA3	1.94	0.49
1:D:9:ILE:CD1	1:D:184:ARG:HH12	2.25	0.49
1:D:36:THR:HG21	1:D:38:ARG:HH11	1.76	0.49
1:B:230:ASN:C	1:B:230:ASN:ND2	2.66	0.49
1:A:230:ASN:ND2	4:A:2023:HOH:O	2.44	0.49
1:C:89:ASN:C	1:C:89:ASN:ND2	2.66	0.49
1:C:28:HIS:CD2	1:C:42:GLN:HE21	2.29	0.49
1:C:279:ASN:CG	1:C:280:LYS:H	2.15	0.49
1:D:185:ILE:O	1:D:185:ILE:CG2	2.60	0.49
1:D:86:ALA:HB3	1:D:97:ASP:HB2	1.95	0.49
1:A:87:TRP:CD1	1:A:93:SER:O	2.66	0.48
1:A:111:GLU:HG2	1:A:112:TYR:N	2.27	0.48
1:D:31:LEU:HD12	1:D:274:ALA:O	2.13	0.48
1:B:180:ALA:CA	3:B:1306:C8E:H81	2.43	0.48
1:B:203:HIS:NE2	1:B:218:LYS:HE3	2.29	0.48
1:D:230:ASN:C	1:D:230:ASN:ND2	2.66	0.48
1:A:85:TYR:CE1	1:A:98:HIS:CD2	3.02	0.48
1:B:203:HIS:CD2	1:B:218:LYS:HG3	2.48	0.48
1:A:187:ASP:O	1:A:233:TYR:HA	2.14	0.48
1:A:81:ASN:OD1	1:A:82:MET:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HG2	1:A:183:TYR:N	2.28	0.48
1:C:9:ILE:N	1:C:14:PHE:CE1	2.72	0.48
1:C:252:GLU:OE2	1:C:254:LYS:HE2	2.13	0.48
1:A:17:ALA:HB3	1:A:56:ASP:HB3	1.94	0.48
1:C:56:ASP:OD2	1:C:57:ILE:N	2.47	0.48
1:B:214:THR:CG2	1:B:260:ILE:HG23	2.44	0.48
1:A:151:ASN:HB3	1:A:154:ALA:HB3	1.95	0.48
1:B:28:HIS:CD2	1:B:44:ASP:OD2	2.66	0.48
1:A:165:VAL:HG12	1:A:166:ILE:HG12	1.95	0.47
1:D:147:SER:HB3	1:D:158:ASN:ND2	2.29	0.47
1:A:31:LEU:HD12	1:A:274:ALA:O	2.14	0.47
1:B:65:LEU:HG	1:B:66:THR:N	2.28	0.47
1:B:122:GLN:HG3	1:B:127:LYS:HE2	1.96	0.47
1:B:246:THR:HB	1:B:283:THR:OG1	2.14	0.47
1:C:166:ILE:HD12	1:C:208:HIS:CE1	2.49	0.47
1:C:222:SER:HB2	4:C:2026:HOH:O	2.14	0.47
1:D:244:GLU:HB3	1:D:285:THR:HG22	1.97	0.47
1:D:33:ASP:O	1:D:37:GLY:N	2.40	0.47
1:C:164:ARG:HH11	1:C:164:ARG:CG	2.28	0.47
1:D:263:ASN:HD22	1:D:264:SER:N	2.12	0.47
1:D:12:ASP:CB	1:D:59:TRP:CH2	2.96	0.47
1:D:43:LEU:CD2	1:D:43:LEU:N	2.77	0.47
1:D:174:MET:HE3	1:D:200:VAL:HG22	1.97	0.47
1:A:7:PRO:HG3	1:A:234:TYR:CE1	2.49	0.47
1:A:179:LEU:N	1:A:179:LEU:HD22	2.30	0.47
1:A:246:THR:O	1:A:282:TYR:HA	2.15	0.47
1:C:9:ILE:CA	1:C:14:PHE:HE1	2.28	0.47
1:A:117:LYS:HE3	1:A:117:LYS:HB2	1.65	0.47
1:B:40:ILE:HG12	1:B:41:SER:N	2.29	0.47
1:C:107:ASN:HB2	1:C:140:SER:HB3	1.95	0.47
1:C:174:MET:HE1	1:C:197:SER:HB3	1.97	0.47
1:B:54:LYS:HA	1:B:72:TRP:HB3	1.96	0.47
1:A:54:LYS:HG2	1:A:72:TRP:HB3	1.95	0.46
1:A:112:TYR:HB2	3:A:1300:C8E:H62	1.98	0.46
1:A:45:TRP:CZ3	1:A:82:MET:HG3	2.50	0.46
1:B:15:THR:O	1:B:57:ILE:HA	2.16	0.46
1:B:252:GLU:OE2	1:B:254:LYS:HE2	2.14	0.46
1:A:202:ALA:HB3	1:A:219:THR:HB	1.97	0.46
1:B:138:ARG:HG2	1:B:171:ARG:HG3	1.96	0.46
1:C:246:THR:O	1:C:282:TYR:HA	2.15	0.46
1:D:68:ASN:OD1	1:D:70:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:CA	3:A:1302:C8E:H81	2.38	0.46
1:C:156:THR:HG22	1:D:9:ILE:H	1.81	0.46
1:D:260:ILE:HG13	1:D:260:ILE:O	2.14	0.46
1:A:48:LYS:O	1:A:49:ASN:C	2.54	0.46
1:B:295:GLY:O	1:B:296:GLY:C	2.54	0.46
1:B:259:THR:O	1:B:267:SER:HA	2.16	0.46
1:D:44:ASP:O	1:D:82:MET:HA	2.16	0.46
1:D:196:PHE:HA	1:D:224:TYR:O	2.15	0.46
1:B:44:ASP:O	1:B:82:MET:HA	2.16	0.46
1:B:117:LYS:HB2	1:B:117:LYS:HE3	1.61	0.46
1:B:174:MET:CE	1:B:200:VAL:HG22	2.46	0.46
1:B:188:PHE:CZ	1:B:231:ALA:HB1	2.50	0.46
1:B:263:ASN:H	1:B:263:ASN:HD22	1.63	0.46
1:A:54:LYS:CE	1:A:244:GLU:OE2	2.64	0.46
1:D:115:ASN:HB2	1:D:176:TYR:OH	2.16	0.46
1:B:174:MET:HE1	1:B:197:SER:HB3	1.97	0.45
1:B:217:GLU:HG2	1:B:275:ALA:HB1	1.98	0.45
1:C:31:LEU:HD12	1:C:274:ALA:O	2.16	0.45
1:D:15:THR:O	1:D:57:ILE:HA	2.16	0.45
1:D:50:VAL:HG12	1:D:51:ALA:O	2.16	0.45
1:C:47:ILE:HG22	1:C:141:TRP:HZ2	1.82	0.45
1:D:246:THR:HB	1:D:283:THR:OG1	2.16	0.45
1:A:49:ASN:ND2	1:A:49:ASN:C	2.70	0.45
1:A:175:PRO:CB	3:A:1303:C8E:H61	2.47	0.45
1:C:164:ARG:HB3	1:C:209:TYR:CD1	2.51	0.45
1:C:230:ASN:ND2	1:C:230:ASN:C	2.69	0.45
1:D:81:ASN:OD1	1:D:82:MET:N	2.50	0.45
1:D:214:THR:CG2	1:D:262:LYS:HD3	2.47	0.45
1:A:206:ASP:OD1	1:A:208:HIS:ND1	2.44	0.45
1:A:87:TRP:CD1	1:A:95:TRP:HA	2.51	0.45
1:A:264:SER:OG	1:A:266:ASP:HB2	2.17	0.45
1:B:47:ILE:HD11	1:B:141:TRP:CZ2	2.52	0.45
1:C:94:GLU:OE1	1:D:123:ASP:HB2	2.16	0.45
1:D:56:ASP:C	1:D:57:ILE:HG13	2.37	0.45
1:D:223:ARG:CG	1:D:251:ASP:OD2	2.64	0.45
1:D:6:ILE:CG2	1:D:7:PRO:HD2	2.46	0.45
1:C:157:GLY:HA2	1:D:7:PRO:O	2.17	0.45
1:D:138:ARG:HG2	1:D:171:ARG:HG3	1.99	0.45
1:D:185:ILE:O	1:D:186:ASN:HB2	2.16	0.45
1:A:107:ASN:HB2	1:A:140:SER:HB3	1.99	0.45
1:B:31:LEU:HB3	1:B:41:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:TYR:CE1	1:D:98:HIS:CD2	3.04	0.45
1:C:156:THR:HG23	1:C:157:GLY:N	2.32	0.45
1:D:87:TRP:CD1	1:D:95:TRP:HA	2.52	0.45
1:A:86:ALA:HB3	1:A:97:ASP:HB2	1.98	0.44
1:A:121:LEU:C	1:A:122:GLN:HG3	2.37	0.44
1:B:24:SER:HA	1:B:47:ILE:O	2.18	0.44
1:C:33:ASP:HB3	1:C:36:THR:HB	1.99	0.44
1:B:261:ASP:HB3	1:B:264:SER:HB2	1.99	0.44
1:C:48:LYS:CE	1:C:81:ASN:HB2	2.46	0.44
1:C:119:TRP:CE3	1:C:127:LYS:HG3	2.52	0.44
1:A:212:ASP:O	1:A:262:LYS:HB2	2.17	0.44
1:C:68:ASN:N	1:C:68:ASN:ND2	2.65	0.44
1:D:9:ILE:HG13	1:D:184:ARG:HH12	1.81	0.44
1:D:107:ASN:HB2	1:D:140:SER:HB3	1.99	0.44
1:D:259:THR:O	1:D:267:SER:HA	2.17	0.44
1:A:8:ASN:HB2	1:A:237:PRO:HB3	1.99	0.44
1:A:185:ILE:O	1:A:185:ILE:HG23	2.17	0.44
1:A:208:HIS:HB3	1:A:211:ARG:HG2	1.99	0.44
1:C:163:VAL:O	1:C:165:VAL:HG23	2.17	0.44
1:D:184:ARG:HA	1:D:188:PHE:O	2.17	0.44
1:D:211:ARG:O	1:D:212:ASP:C	2.54	0.44
1:C:267:SER:O	1:C:268:VAL:CG2	2.58	0.44
1:A:138:ARG:HG2	1:A:171:ARG:HG3	1.98	0.44
1:B:59:TRP:HH2	1:B:296:GLY:O	2.00	0.44
1:B:125:ASN:C	1:B:126:TYR:CD1	2.91	0.44
1:B:174:MET:HB2	1:B:174:MET:HE2	1.73	0.44
1:C:174:MET:HB2	1:C:174:MET:HE2	1.70	0.44
1:C:201:ARG:NH2	4:C:2020:HOH:O	2.50	0.44
1:A:5:LEU:O	1:A:187:ASP:HB3	2.17	0.44
1:B:190:LEU:HD12	1:B:230:ASN:O	2.18	0.44
1:C:43:LEU:HA	1:C:83:ASP:O	2.18	0.44
1:C:219:THR:CG2	1:C:253:GLY:HA3	2.47	0.44
1:B:126:TYR:CE2	1:B:183:TYR:CD1	3.06	0.44
1:C:28:HIS:HD2	1:C:44:ASP:OD2	2.01	0.44
1:C:33:ASP:OD1	1:C:33:ASP:C	2.56	0.44
1:A:8:ASN:ND2	4:A:2001:HOH:O	2.28	0.43
1:C:187:ASP:O	1:C:188:PHE:HB2	2.16	0.43
1:D:203:HIS:CE1	2:D:1297:SO4:O4	2.71	0.43
1:A:184:ARG:O	1:A:185:ILE:HB	2.18	0.43
1:C:74:SER:HB2	1:C:109:ALA:H	1.83	0.43
1:A:122:GLN:HE21	1:A:122:GLN:HB2	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LEU:HD23	1:D:191:ASN:N	2.34	0.43
1:A:125:ASN:O	1:A:183:TYR:HA	2.18	0.43
1:B:194:PHE:HE2	1:B:196:PHE:CD1	2.32	0.43
1:C:117:LYS:HE3	1:C:117:LYS:HB2	1.63	0.43
1:C:121:LEU:O	1:C:127:LYS:HB2	2.18	0.43
1:C:135:GLN:HE21	1:C:135:GLN:HB3	1.65	0.43
1:A:127:LYS:HE3	1:A:127:LYS:HB2	1.87	0.43
1:A:252:GLU:OE2	1:A:254:LYS:HE2	2.19	0.43
1:A:54:LYS:HG3	1:A:72:TRP:CB	2.47	0.43
1:A:245:PHE:CE1	1:A:282:TYR:HB2	2.54	0.43
1:B:191:ASN:N	1:B:191:ASN:ND2	2.66	0.43
1:B:263:ASN:HD22	1:B:263:ASN:N	2.17	0.43
1:C:156:THR:HG21	1:D:9:ILE:HG12	2.00	0.43
1:A:115:ASN:HB2	1:A:176:TYR:OH	2.19	0.43
1:A:246:THR:HB	1:A:283:THR:OG1	2.19	0.43
1:D:148:TYR:CZ	1:D:157:GLY:CA	3.00	0.43
1:D:204:ASP:OD1	1:D:204:ASP:C	2.58	0.43
1:A:87:TRP:HD1	1:A:93:SER:O	2.02	0.42
1:A:273:ASP:N	1:A:273:ASP:OD2	2.51	0.42
1:B:14:PHE:CD2	1:B:59:TRP:CE3	3.07	0.42
1:D:174:MET:HE2	1:D:200:VAL:HG22	2.02	0.42
1:C:54:LYS:HG3	1:C:72:TRP:HB3	2.01	0.42
1:B:185:ILE:HD13	1:B:186:ASN:OD1	2.20	0.42
1:B:188:PHE:C	1:B:188:PHE:HD2	2.22	0.42
1:C:206:ASP:HB3	1:C:215:PHE:HB2	1.99	0.42
1:A:222:SER:HB2	4:A:2027:HOH:O	2.18	0.42
1:B:160:PRO:HB2	1:B:163:VAL:HG23	2.02	0.42
1:B:203:HIS:CE1	4:B:2016:HOH:O	2.72	0.42
1:C:166:ILE:HD12	1:C:208:HIS:CD2	2.54	0.42
1:A:166:ILE:HD12	1:A:208:HIS:NE2	2.34	0.42
1:A:217:GLU:HB3	1:A:277:ILE:HD11	2.00	0.42
1:B:14:PHE:CE2	1:B:59:TRP:CE3	3.07	0.42
1:B:107:ASN:HB2	1:B:140:SER:HB3	2.01	0.42
1:C:13:SER:CB	1:C:59:TRP:CZ3	2.82	0.42
1:C:156:THR:CG2	1:D:7:PRO:O	2.67	0.42
1:D:15:THR:HG22	1:D:58:SER:N	2.35	0.42
1:A:112:TYR:CB	3:A:1300:C8E:H62	2.50	0.42
1:A:166:ILE:HD12	1:A:208:HIS:CD2	2.55	0.42
1:C:61:PRO:HB2	1:C:62:TYR:CE1	2.54	0.42
1:D:89:ASN:CB	1:D:92:GLN:HB3	2.37	0.42
1:A:174:MET:HE3	1:A:200:VAL:HG22	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ILE:HD11	1:C:196:PHE:HD1	1.84	0.42
1:B:81:ASN:OD1	1:B:82:MET:N	2.51	0.42
1:B:125:ASN:OD1	1:B:184:ARG:O	2.38	0.42
1:D:33:ASP:HB3	1:D:36:THR:HB	2.02	0.42
1:D:74:SER:HB2	1:D:109:ALA:H	1.85	0.42
1:D:202:ALA:O	1:D:218:LYS:HA	2.20	0.42
1:C:38:ARG:HE	1:C:90:GLU:CG	2.30	0.42
1:C:57:ILE:HD13	1:C:58:SER:N	2.35	0.42
1:A:74:SER:HB2	1:A:109:ALA:H	1.85	0.41
1:B:275:ALA:HB1	3:B:1304:C8E:H11	2.02	0.41
1:D:59:TRP:CD1	1:D:67:LEU:HD12	2.55	0.41
1:A:174:MET:HA	1:A:175:PRO:HD3	1.95	0.41
1:B:34:ALA:HB1	1:B:272:GLY:O	2.20	0.41
1:B:174:MET:HA	1:B:175:PRO:HD3	1.94	0.41
1:D:147:SER:O	1:D:159:PHE:HE1	2.04	0.41
1:A:238:ASN:ND2	2:A:1295:SO4:O4	2.54	0.41
1:A:270:ILE:CG2	1:A:271:GLY:N	2.83	0.41
1:B:29:GLU:HB3	1:B:43:LEU:HB2	2.01	0.41
1:B:43:LEU:N	1:B:43:LEU:CD2	2.83	0.41
1:B:164:ARG:CG	1:B:164:ARG:NH1	2.59	0.41
1:C:40:ILE:O	1:C:86:ALA:HA	2.20	0.41
1:B:122:GLN:HG3	1:B:127:LYS:HB3	2.02	0.41
1:C:34:ALA:HB2	1:C:274:ALA:HB2	2.02	0.41
1:D:29:GLU:HB3	1:D:43:LEU:HB2	2.01	0.41
1:D:50:VAL:HG22	1:D:78:GLY:HA3	2.01	0.41
1:D:203:HIS:CD2	1:D:218:LYS:HG2	2.55	0.41
1:B:187:ASP:O	1:B:233:TYR:HA	2.20	0.41
1:D:281:ASN:HD22	1:D:281:ASN:HA	1.65	0.41
1:B:188:PHE:HE2	1:B:190:LEU:HB2	1.86	0.41
1:D:15:THR:CG2	1:D:58:SER:HB3	2.50	0.41
1:D:74:SER:CB	1:D:109:ALA:H	2.34	0.41
1:D:214:THR:CG2	1:D:260:ILE:HG23	2.47	0.41
1:D:227:THR:HG23	1:D:247:TYR:HB3	2.03	0.41
1:A:43:LEU:N	1:A:43:LEU:CD2	2.84	0.41
1:A:204:ASP:OD1	1:A:217:GLU:OE1	2.38	0.41
1:C:164:ARG:HD3	2:C:1298:SO4:O2	2.20	0.41
1:A:125:ASN:OD1	1:A:125:ASN:N	2.53	0.41
1:B:17:ALA:O	1:B:56:ASP:N	2.49	0.41
1:B:74:SER:HB2	1:B:109:ALA:H	1.85	0.41
1:B:185:ILE:CG2	1:B:188:PHE:HB3	2.51	0.41
1:B:214:THR:HG22	1:B:260:ILE:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASN:HB2	1:B:176:TYR:OH	2.21	0.41
1:C:214:THR:HB	1:C:260:ILE:HG23	2.02	0.41
1:D:117:LYS:HE3	1:D:117:LYS:HB2	1.72	0.41
1:B:56:ASP:OD2	1:B:68:ASN:ND2	2.54	0.41
1:C:130:ILE:HG22	1:C:179:LEU:HD13	2.02	0.41
1:C:130:ILE:HG22	1:C:179:LEU:CD1	2.51	0.40
1:D:262:LYS:HE2	1:D:262:LYS:HB3	1.86	0.40
1:B:61:PRO:O	1:B:297:GLY:CA	2.69	0.40
1:C:54:LYS:NZ	1:C:70:ARG:HH12	2.20	0.40
1:C:174:MET:CE	1:C:224:TYR:HB3	2.52	0.40
1:C:200:VAL:HG23	1:C:222:SER:O	2.21	0.40
1:D:23:LEU:HG	1:D:47:ILE:CD1	2.52	0.40
1:D:87:TRP:CE2	1:D:95:TRP:HB3	2.56	0.40
1:C:81:ASN:OD1	1:C:82:MET:N	2.54	0.40
1:D:204:ASP:OD1	1:D:217:GLU:OE1	2.40	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.90	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASP:OD2	1:C:97:ASP:OD2[2_544]	2.10	0.10
1:B:97:ASP:OD2	1:C:266:ASP:OD2[2_544]	2.14	0.06
1:A:266:ASP:OD2	1:D:97:ASP:OD2[2_554]	2.18	0.02

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	291/298 (98%)	267 (92%)	18 (6%)	6 (2%)	7 7
1	B	284/298 (95%)	261 (92%)	16 (6%)	7 (2%)	5 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	289/298 (97%)	263 (91%)	14 (5%)	12 (4%)	3 1
1	D	291/298 (98%)	269 (92%)	15 (5%)	7 (2%)	6 5
All	All	1155/1192 (97%)	1060 (92%)	63 (6%)	32 (3%)	5 4

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	185	ILE
1	A	264	SER
1	B	49	ASN
1	C	5	LEU
1	C	7	PRO
1	C	10	SER
1	C	188	PHE
1	C	268	VAL
1	D	12	ASP
1	A	49	ASN
1	A	272	GLY
1	C	11	PRO
1	C	13	SER
1	C	92	GLN
1	D	293	GLY
1	A	266	ASP
1	B	123	ASP
1	B	125	ASN
1	C	124	GLU
1	C	273	ASP
1	D	11	PRO
1	D	263	ASN
1	B	186	ASN
1	B	296	GLY
1	D	3	SER
1	C	4	GLN
1	D	61	PRO
1	D	212	ASP
1	B	272	GLY
1	C	6	ILE
1	B	295	GLY

5.3.2 Protein sidechains (i)

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	239/240 (100%)	209 (87%)	30 (13%)	4 4
1	B	229/240 (95%)	192 (84%)	37 (16%)	2 2
1	C	229/240 (95%)	189 (82%)	40 (18%)	2 2
1	D	239/240 (100%)	202 (84%)	37 (16%)	2 2
All	All	936/960 (98%)	792 (85%)	144 (15%)	2 2

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	15	THR
1	A	24	SER
1	A	30	MET
1	A	38	ARG
1	A	40	ILE
1	A	43	LEU
1	A	48	LYS
1	A	49	ASN
1	A	66	THR
1	A	68	ASN
1	A	110	ASN
1	A	111	GLU
1	A	115	ASN
1	A	120	LEU
1	A	122	GLN
1	A	125	ASN
1	A	156	THR
1	A	164	ARG
1	A	169	ASN
1	A	171	ARG
1	A	173	SER
1	A	174	MET
1	A	207	GLU

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Mol	Chain	Res	Type
1	A	216	ARG
1	A	219	THR
1	A	224	TYR
1	A	230	ASN
1	A	246	THR
1	A	285	THR
1	B	15	THR
1	B	24	SER
1	B	30	MET
1	B	40	ILE
1	B	43	LEU
1	B	58	SER
1	B	66	THR
1	B	70	ARG
1	B	110	ASN
1	B	111	GLU
1	B	115	ASN
1	B	120	LEU
1	B	123	ASP
1	B	124	GLU
1	B	156	THR
1	B	164	ARG
1	B	169	ASN
1	B	171	ARG
1	B	173	SER
1	B	174	MET
1	B	182	GLN
1	B	185	ILE
1	B	190	LEU
1	B	191	ASN
1	B	193	LEU
1	B	196	PHE
1	B	214	THR
1	B	219	THR
1	B	224	TYR
1	B	227	THR
1	B	230	ASN
1	B	246	THR
1	B	260	ILE
1	B	282	TYR
1	B	285	THR
1	B	291	ARG

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Mol	Chain	Res	Type
1	B	292	PHE
1	C	15	THR
1	C	24	SER
1	C	30	MET
1	C	35	GLU
1	C	38	ARG
1	C	40	ILE
1	C	43	LEU
1	C	47	ILE
1	C	48	LYS
1	C	52	ILE
1	C	57	ILE
1	C	60	ASP
1	C	62	TYR
1	C	66	THR
1	C	67	LEU
1	C	70	ARG
1	C	89	ASN
1	C	110	ASN
1	C	111	GLU
1	C	115	ASN
1	C	156	THR
1	C	163	VAL
1	C	164	ARG
1	C	169	ASN
1	C	171	ARG
1	C	173	SER
1	C	174	MET
1	C	175	PRO
1	C	177	ILE
1	C	191	ASN
1	C	193	LEU
1	C	211	ARG
1	C	214	THR
1	C	218	LYS
1	C	219	THR
1	C	222	SER
1	C	230	ASN
1	C	246	THR
1	C	260	ILE
1	C	285	THR
1	D	3	SER

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Mol	Chain	Res	Type
1	D	6	ILE
1	D	15	THR
1	D	22	MET
1	D	24	SER
1	D	30	MET
1	D	36	THR
1	D	43	LEU
1	D	47	ILE
1	D	48	LYS
1	D	66	THR
1	D	68	ASN
1	D	92	GLN
1	D	110	ASN
1	D	111	GLU
1	D	115	ASN
1	D	120	LEU
1	D	124	GLU
1	D	149	SER
1	D	156	THR
1	D	164	ARG
1	D	169	ASN
1	D	171	ARG
1	D	173	SER
1	D	174	MET
1	D	193	LEU
1	D	196	PHE
1	D	198	ASP
1	D	211	ARG
1	D	220	SER
1	D	222	SER
1	D	227	THR
1	D	230	ASN
1	D	246	THR
1	D	260	ILE
1	D	263	ASN
1	D	285	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	98	HIS

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	108	HIS
1	A	110	ASN
1	A	158	ASN
1	A	186	ASN
1	A	205	ASN
1	A	230	ASN
1	A	281	ASN
1	B	28	HIS
1	B	98	HIS
1	B	107	ASN
1	B	110	ASN
1	B	122	GLN
1	B	182	GLN
1	B	191	ASN
1	B	230	ASN
1	B	263	ASN
1	B	281	ASN
1	C	28	HIS
1	C	49	ASN
1	C	89	ASN
1	C	107	ASN
1	C	110	ASN
1	C	125	ASN
1	C	182	GLN
1	C	230	ASN
1	C	263	ASN
1	C	281	ASN
1	D	28	HIS
1	D	98	HIS
1	D	107	ASN
1	D	110	ASN
1	D	152	ASN
1	D	158	ASN
1	D	203	HIS
1	D	230	ASN
1	D	263	ASN
1	D	281	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

37 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	SO4	B	1302	-	4,4,4	0.12	0	6,6,6	0.30	0
3	C8E	B	1305	-	7,7,20	0.33	0	6,6,19	0.43	0
3	C8E	D	1304	-	8,8,20	0.34	0	7,7,19	0.37	0
2	SO4	D	1296	-	4,4,4	0.14	0	6,6,6	0.08	0
3	C8E	C	1300	-	10,10,20	0.39	0	9,9,19	0.38	0
3	C8E	D	1302	-	11,11,20	0.34	0	10,10,19	0.49	0
2	SO4	A	1295	-	4,4,4	0.12	0	6,6,6	0.18	0
3	C8E	B	1304	-	7,7,20	0.31	0	6,6,19	0.44	0
2	SO4	B	1301	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	D	1300	-	4,4,4	0.10	0	6,6,6	0.25	0
2	SO4	C	1297	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	A	1298	-	4,4,4	0.16	0	6,6,6	0.15	0
3	C8E	A	1301	-	8,8,20	0.32	0	7,7,19	0.53	0
3	C8E	C	1302	-	8,8,20	0.36	0	7,7,19	0.46	0
3	C8E	D	1303	-	8,8,20	0.31	0	7,7,19	0.46	0
3	C8E	C	1301	-	8,8,20	0.36	0	7,7,19	0.38	0
2	SO4	A	1299	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	D	1298	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	C	1296	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	D	1301	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	C	1298	-	4,4,4	0.17	0	6,6,6	0.33	0
3	C8E	A	1303	-	9,9,20	0.36	0	8,8,19	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	1299	-	4,4,4	0.06	0	6,6,6	0.32	0
3	C8E	A	1300	-	10,10,20	0.37	0	9,9,19	0.46	0
2	SO4	B	1303	-	4,4,4	0.18	0	6,6,6	0.34	0
2	SO4	D	1299	-	4,4,4	0.08	0	6,6,6	0.23	0
2	SO4	C	1295	-	4,4,4	0.08	0	6,6,6	0.34	0
3	C8E	A	1302	-	8,8,20	0.35	0	7,7,19	0.34	0
2	SO4	A	1297	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	C	1299	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	B	1300	-	4,4,4	0.19	0	6,6,6	0.29	0
3	C8E	A	1304	-	7,7,20	0.39	0	6,6,19	0.18	0
2	SO4	A	1296	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	D	1295	-	4,4,4	0.17	0	6,6,6	0.12	0
3	C8E	B	1306	-	10,10,20	0.34	0	9,9,19	0.40	0
2	SO4	D	1297	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	C	1294	-	4,4,4	0.20	0	6,6,6	0.35	0

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
3	C8E	B	1305	-	-	3/5/5/18	-
3	C8E	D	1303	-	-	5/6/6/18	-
3	C8E	C	1300	-	-	5/8/8/18	-
3	C8E	D	1302	-	-	5/9/9/18	-
3	C8E	D	1304	-	-	4/6/6/18	-
3	C8E	C	1301	-	-	1/6/6/18	-
3	C8E	B	1304	-	-	4/5/5/18	-
3	C8E	A	1304	-	-	2/5/5/18	-
3	C8E	B	1306	-	-	6/8/8/18	-
3	C8E	A	1303	-	-	4/7/7/18	-
3	C8E	A	1301	-	-	2/6/6/18	-
3	C8E	A	1302	-	-	5/6/6/18	-
3	C8E	C	1302	-	-	1/6/6/18	-
3	C8E	A	1300	-	-	7/8/8/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	C8E	C3-C4-C5-C6
3	B	1306	C8E	C4-C5-C6-C7
3	A	1300	C8E	C6-C7-C8-O9
3	B	1304	C8E	C2-C3-C4-C5
3	D	1304	C8E	C4-C5-C6-C7
3	A	1302	C8E	C2-C3-C4-C5
3	D	1303	C8E	C2-C3-C4-C5
3	C	1300	C8E	C3-C4-C5-C6
3	B	1306	C8E	C3-C4-C5-C6
3	D	1302	C8E	C2-C3-C4-C5
3	A	1300	C8E	C3-C4-C5-C6
3	A	1300	C8E	C5-C6-C7-C8
3	D	1302	C8E	C5-C6-C7-C8
3	A	1303	C8E	C7-C8-O9-C10
3	C	1300	C8E	C1-C2-C3-C4
3	A	1302	C8E	C5-C6-C7-C8
3	B	1306	C8E	O9-C10-C11-O12
3	D	1302	C8E	O9-C10-C11-O12
3	A	1302	C8E	C1-C2-C3-C4
3	B	1305	C8E	C5-C6-C7-C8
3	A	1300	C8E	C1-C2-C3-C4
3	D	1304	C8E	C1-C2-C3-C4
3	B	1304	C8E	C3-C4-C5-C6
3	A	1304	C8E	C1-C2-C3-C4
3	C	1301	C8E	C6-C7-C8-O9
3	B	1306	C8E	C6-C7-C8-O9
3	C	1300	C8E	C4-C5-C6-C7
3	C	1300	C8E	C5-C6-C7-C8
3	D	1304	C8E	C6-C7-C8-O9
3	A	1301	C8E	C2-C3-C4-C5
3	D	1303	C8E	C3-C4-C5-C6
3	B	1305	C8E	C6-C7-C8-O9
3	D	1302	C8E	C4-C5-C6-C7
3	B	1306	C8E	C5-C6-C7-C8
3	A	1303	C8E	C1-C2-C3-C4
3	A	1303	C8E	C6-C7-C8-O9
3	D	1304	C8E	C2-C3-C4-C5
3	C	1302	C8E	C2-C3-C4-C5
3	B	1304	C8E	C4-C5-C6-C7
3	D	1303	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	B	1306	C8E	C2-C3-C4-C5
3	B	1304	C8E	C5-C6-C7-C8
3	D	1303	C8E	C6-C7-C8-O9
3	D	1303	C8E	C1-C2-C3-C4
3	A	1301	C8E	C1-C2-C3-C4
3	A	1302	C8E	C6-C7-C8-O9
3	A	1300	C8E	C11-C10-O9-C8
3	A	1302	C8E	C3-C4-C5-C6
3	C	1300	C8E	C2-C3-C4-C5
3	B	1305	C8E	C2-C3-C4-C5
3	A	1300	C8E	C4-C5-C6-C7
3	D	1302	C8E	C3-C4-C5-C6
3	A	1300	C8E	C2-C3-C4-C5
3	A	1304	C8E	C3-C4-C5-C6

There are no ring outliers.

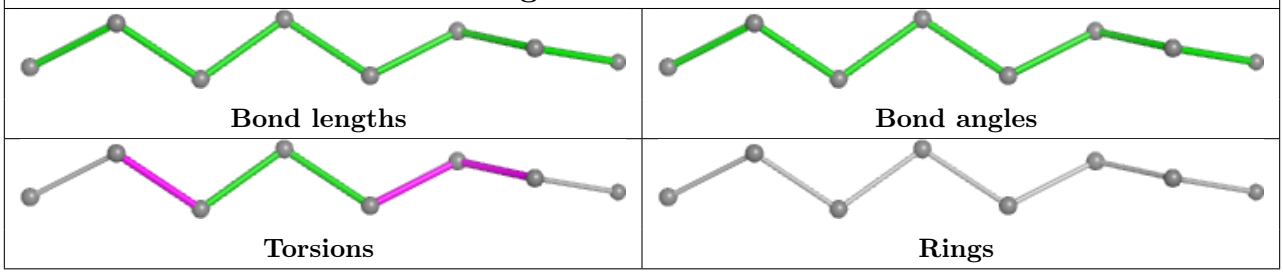
14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1302	SO4	2	0
2	D	1296	SO4	1	0
2	A	1295	SO4	1	0
3	B	1304	C8E	1	0
2	C	1298	SO4	1	0
3	A	1303	C8E	3	0
3	A	1300	C8E	2	0
2	B	1303	SO4	1	0
2	C	1295	SO4	1	0
3	A	1302	C8E	2	0
2	A	1296	SO4	1	0
3	B	1306	C8E	2	0
2	D	1297	SO4	1	0
2	C	1294	SO4	1	0

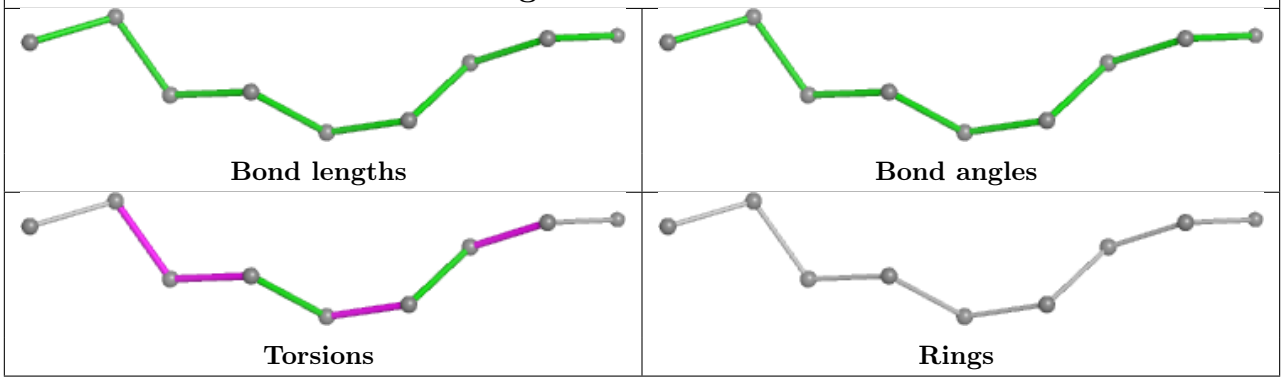
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

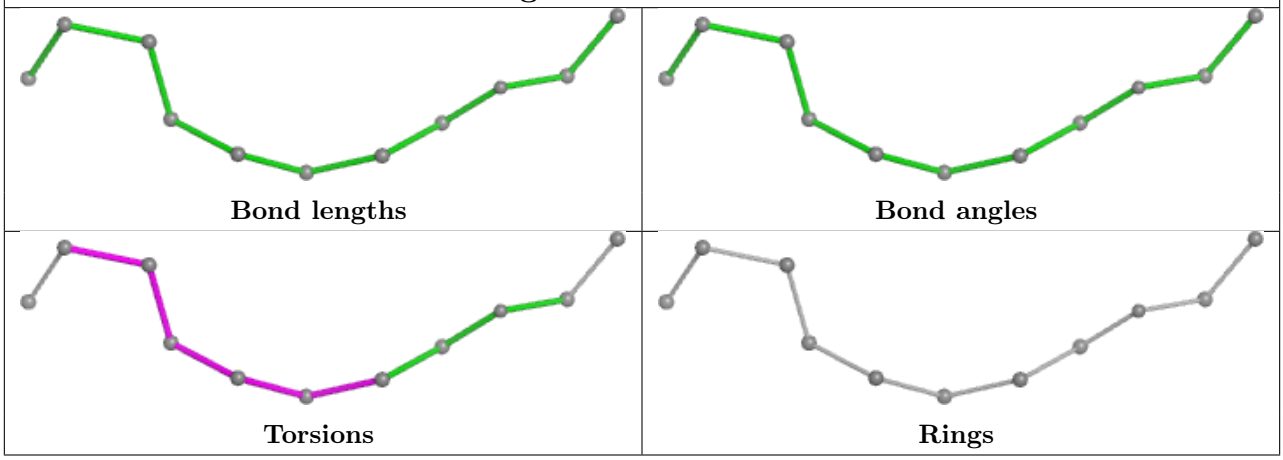
Ligand C8E B 1305



Ligand C8E D 1304



Ligand C8E C 1300



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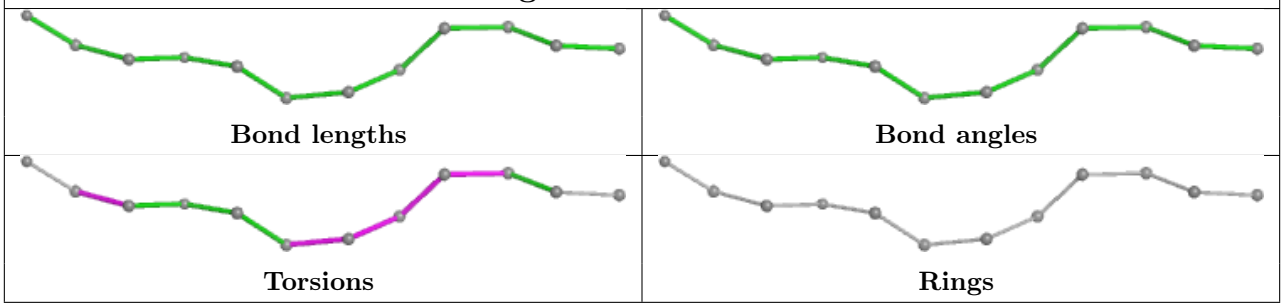
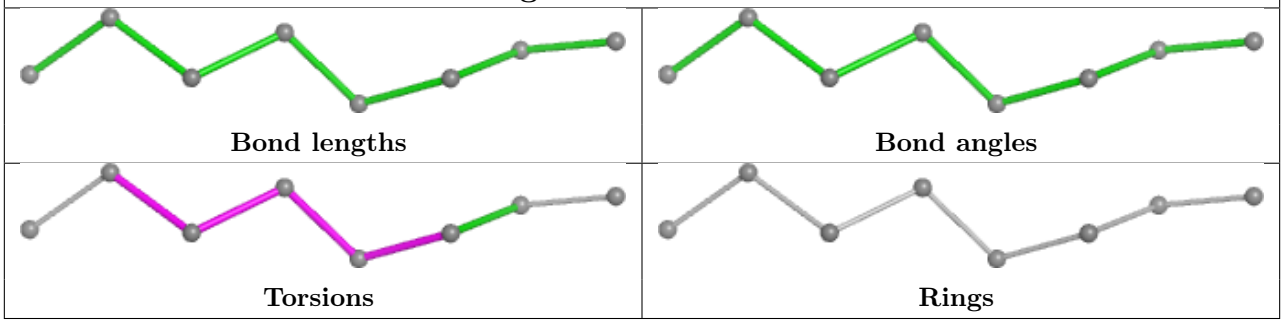
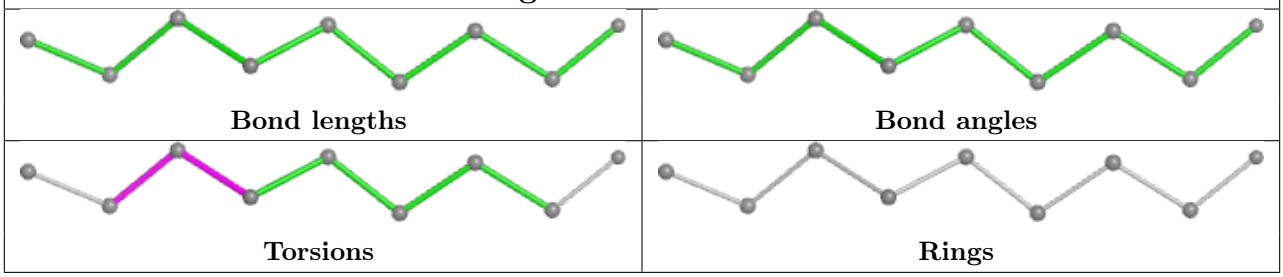


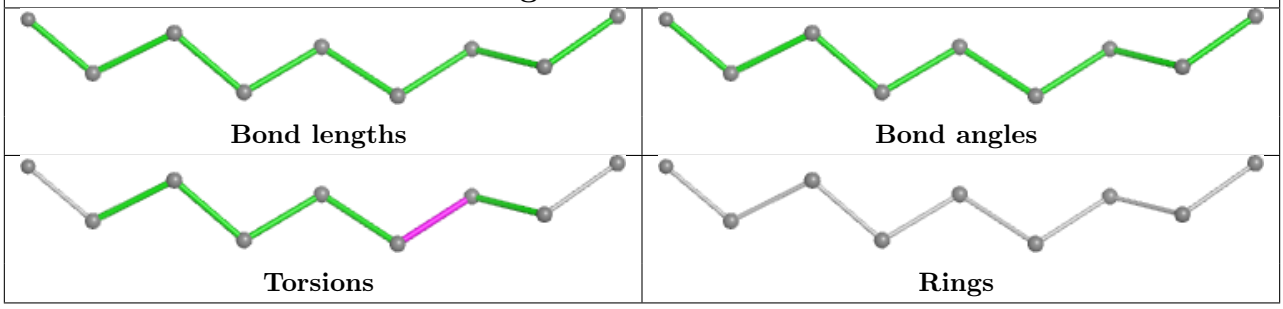
Ligand C8E B 1304



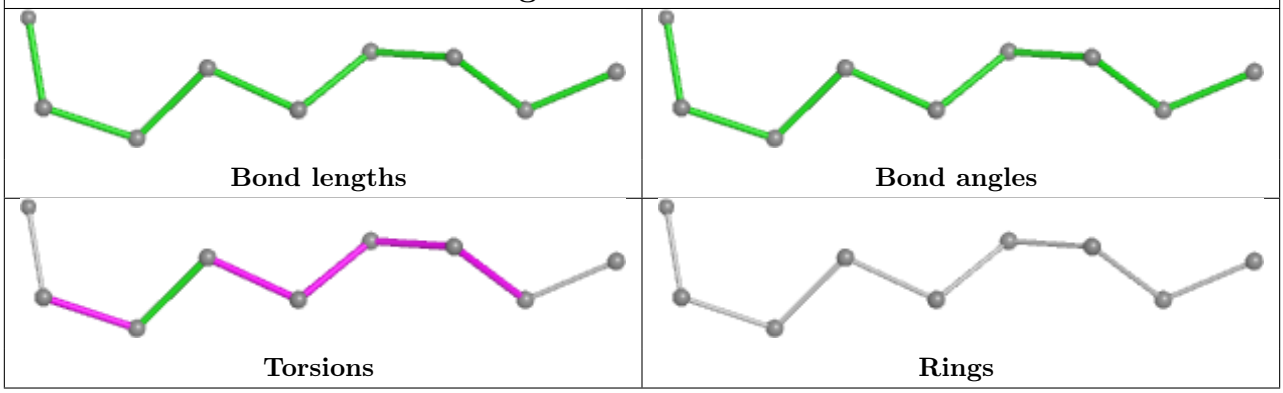
Ligand C8E A 1301



Ligand C8E C 1302



Ligand C8E D 1303



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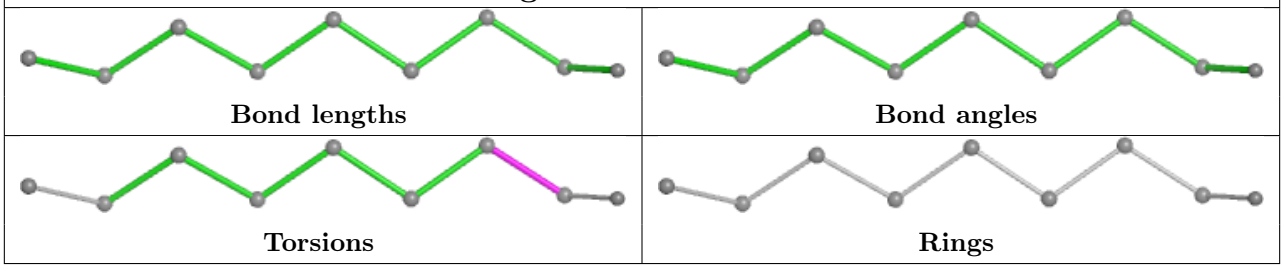
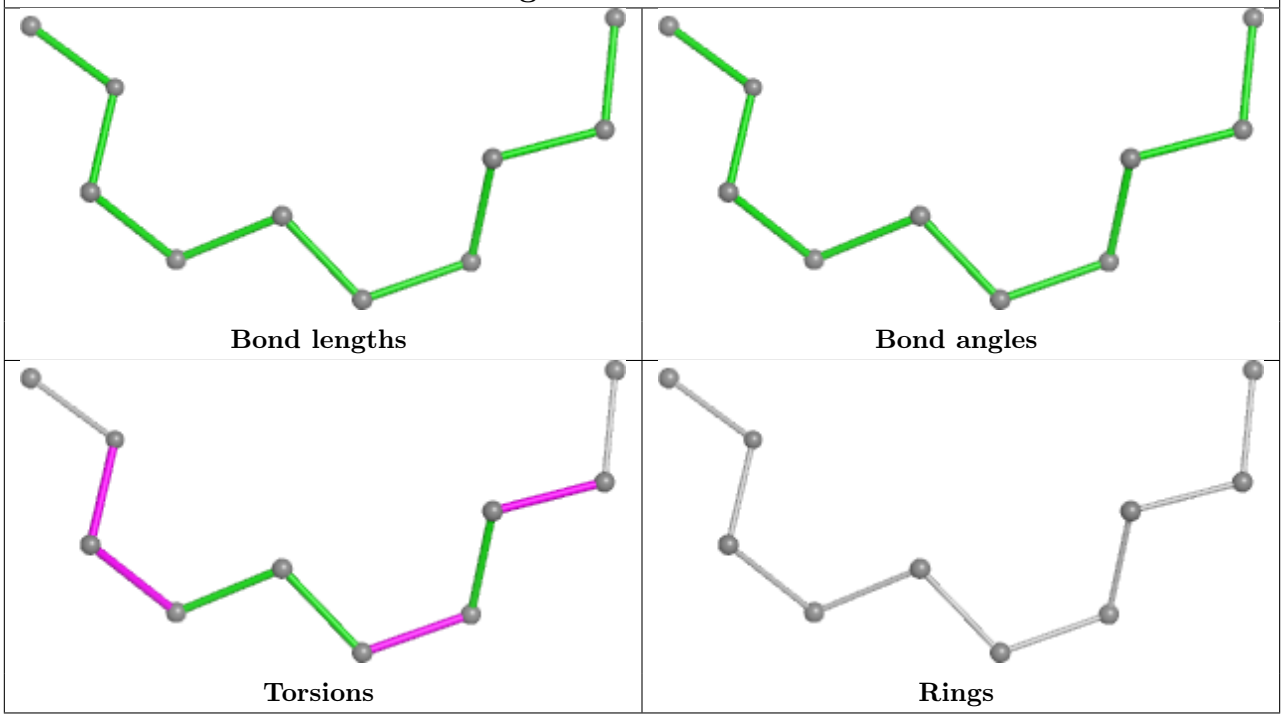
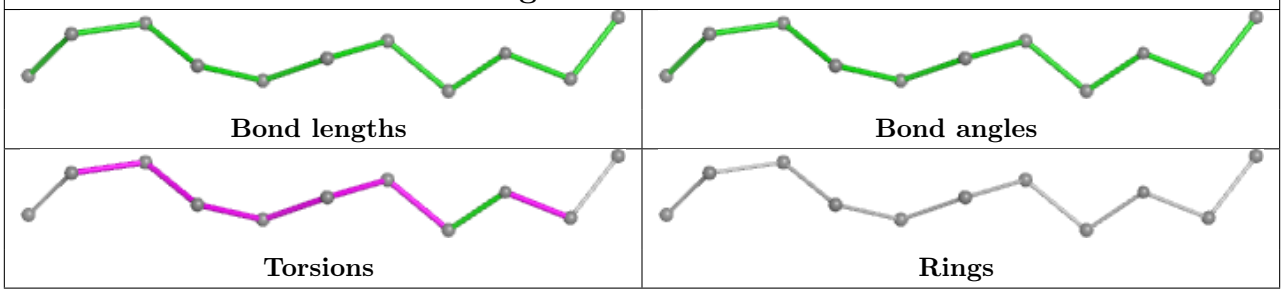


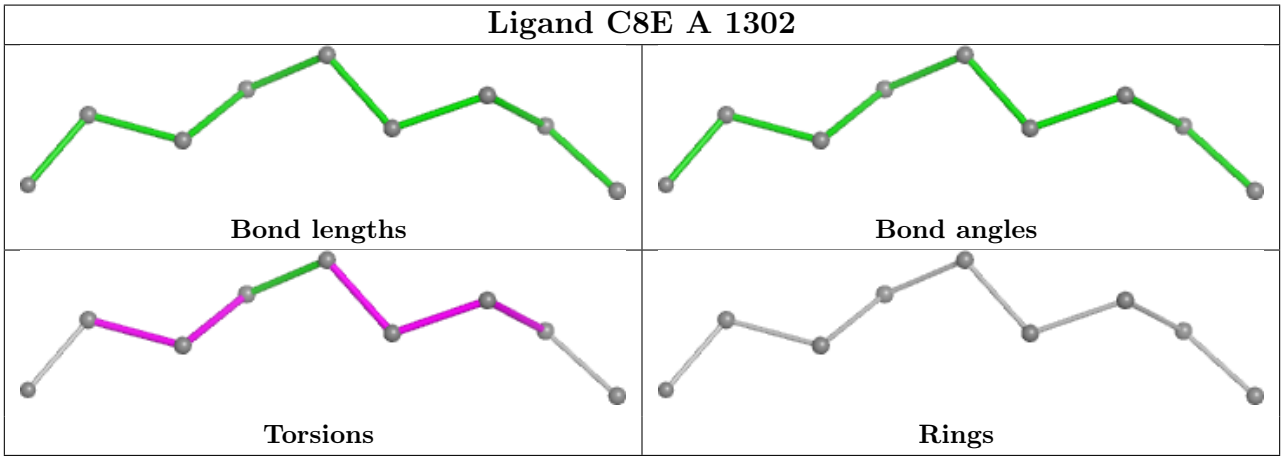
Ligand C8E A 1303

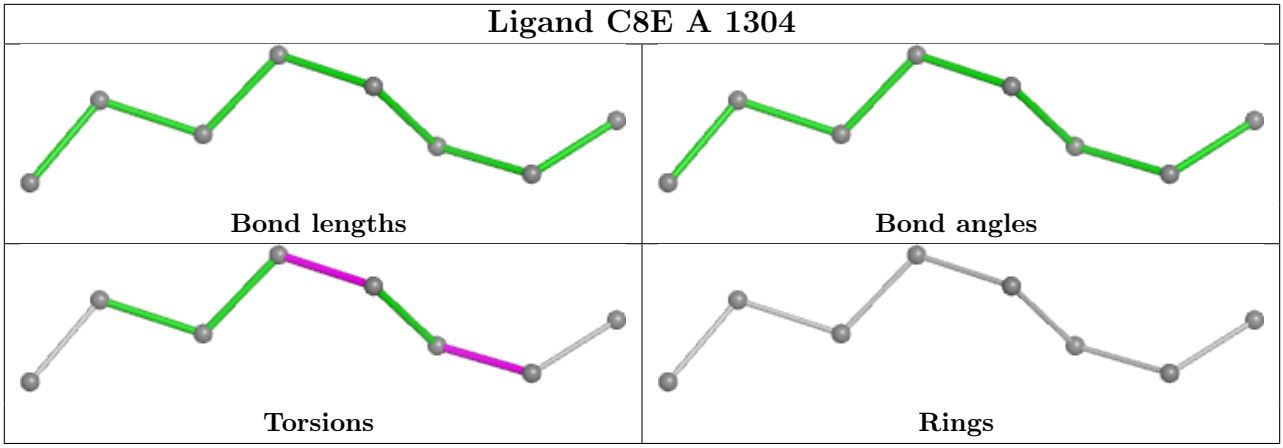


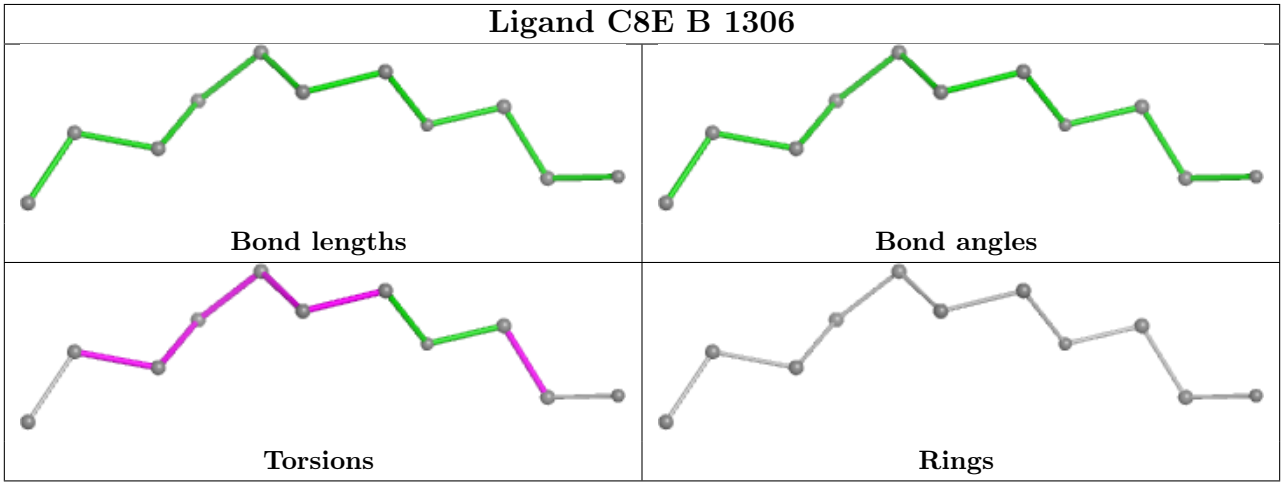
Ligand C8E A 1300



Ligand C8E A 1302







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	293/298 (98%)	0.12	0 100 100	36, 48, 63, 76	0
1	B	286/298 (95%)	0.23	12 (4%) 36 42	34, 50, 77, 97	0
1	C	291/298 (97%)	0.18	5 (1%) 70 76	35, 49, 74, 91	0
1	D	293/298 (98%)	0.08	1 (0%) 94 96	31, 49, 66, 92	0
All	All	1163/1192 (97%)	0.15	18 (1%) 73 79	31, 49, 71, 97	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	SER	4.4
1	C	235	VAL	3.8
1	B	291	ARG	3.7
1	B	63	SER	3.6
1	B	282	TYR	3.5
1	B	235	VAL	3.5
1	B	14	PHE	3.0
1	B	246	THR	3.0
1	B	292	PHE	2.9
1	C	282	TYR	2.3
1	B	247	TYR	2.3
1	C	8	ASN	2.2
1	B	194	PHE	2.2
1	B	227	THR	2.1
1	B	62	TYR	2.1
1	B	155	TYR	2.1
1	D	2	SER	2.0
1	C	17	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	SO4	B	1301	5/5	0.82	0.23	79,80,99,110	0
3	C8E	A	1304	8/21	0.82	0.26	36,43,46,48	0
3	C8E	B	1306	11/21	0.83	0.51	47,54,62,63	0
3	C8E	A	1300	11/21	0.87	0.28	39,49,68,68	0
2	SO4	A	1299	5/5	0.88	0.12	49,64,85,96	0
2	SO4	D	1297	5/5	0.88	0.19	74,76,85,100	0
2	SO4	D	1299	5/5	0.88	0.16	72,91,94,101	0
3	C8E	C	1300	11/21	0.88	0.19	41,43,49,51	0
3	C8E	D	1302	12/21	0.88	0.22	39,50,68,71	0
3	C8E	D	1304	9/21	0.89	0.20	34,49,52,56	0
3	C8E	C	1302	9/21	0.90	0.15	37,41,48,57	0
3	C8E	A	1303	10/21	0.90	0.14	37,42,46,58	0
3	C8E	D	1303	9/21	0.90	0.23	40,46,63,67	0
3	C8E	B	1305	8/21	0.90	0.15	32,40,45,47	0
2	SO4	B	1303	5/5	0.91	0.14	55,57,65,72	0
3	C8E	B	1304	8/21	0.91	0.20	36,40,46,46	0
2	SO4	C	1294	5/5	0.91	0.17	69,70,84,84	0
2	SO4	A	1295	5/5	0.92	0.17	61,74,93,105	0
3	C8E	A	1301	9/21	0.92	0.25	39,45,49,58	0
2	SO4	B	1300	5/5	0.93	0.14	58,73,75,79	0
2	SO4	B	1302	5/5	0.93	0.19	43,61,70,70	0
3	C8E	A	1302	9/21	0.93	0.23	40,44,53,62	0
3	C8E	C	1301	9/21	0.93	0.21	39,46,56,63	0
2	SO4	D	1300	5/5	0.94	0.18	56,62,83,84	0
2	SO4	C	1297	5/5	0.94	0.12	65,67,79,86	0
2	SO4	D	1296	5/5	0.94	0.14	62,67,72,79	0
2	SO4	A	1296	5/5	0.95	0.17	64,66,83,91	0

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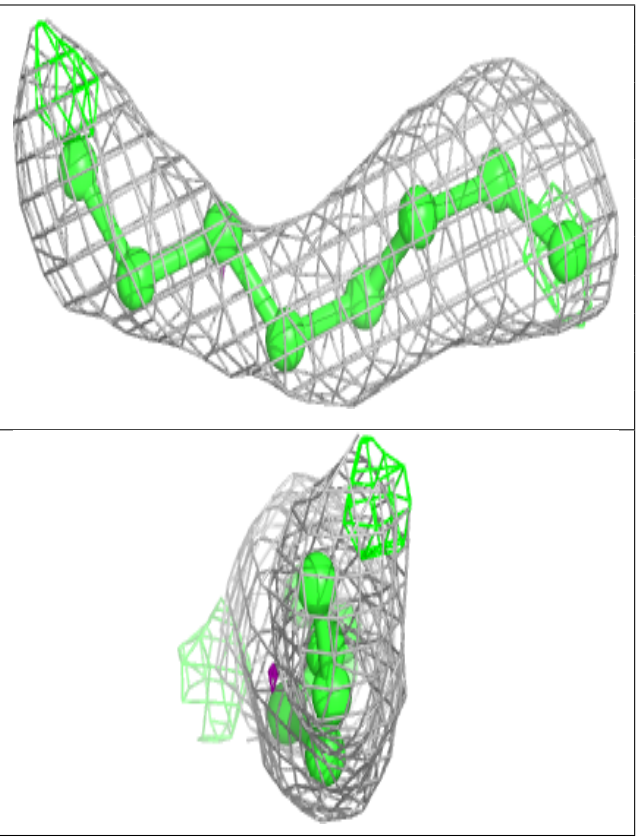
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1299	5/5	0.95	0.17	43,69,78,78	0
2	SO4	C	1298	5/5	0.95	0.28	45,49,64,65	0
2	SO4	D	1301	5/5	0.96	0.13	46,66,79,84	0
2	SO4	C	1299	5/5	0.96	0.14	49,63,72,75	0
2	SO4	D	1298	5/5	0.96	0.11	69,75,83,87	0
2	SO4	D	1295	5/5	0.97	0.28	61,74,82,90	0
2	SO4	C	1296	5/5	0.97	0.14	38,56,70,72	0
2	SO4	A	1298	5/5	0.97	0.14	56,62,77,82	0
2	SO4	C	1295	5/5	0.98	0.13	41,51,51,52	0
2	SO4	A	1297	5/5	0.98	0.18	57,70,77,84	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.

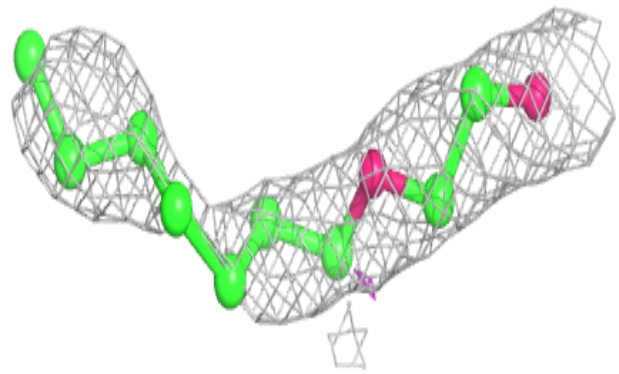
Electron density around C8E A 1304:

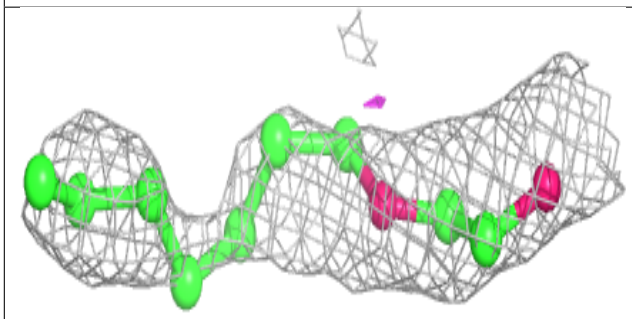
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

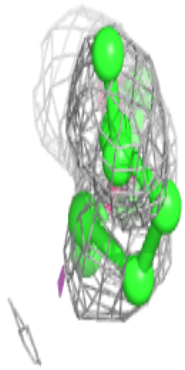


Electron density around C8E B 1306:

$2mF_o$-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 1300:

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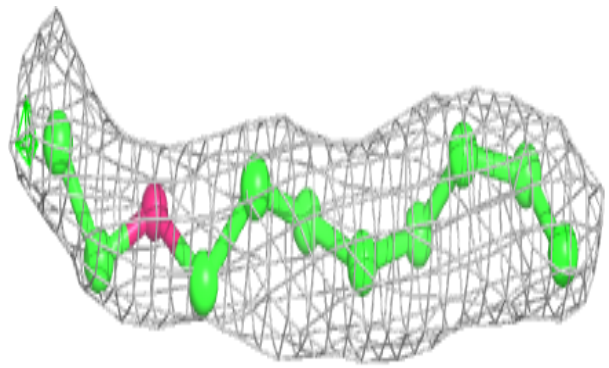
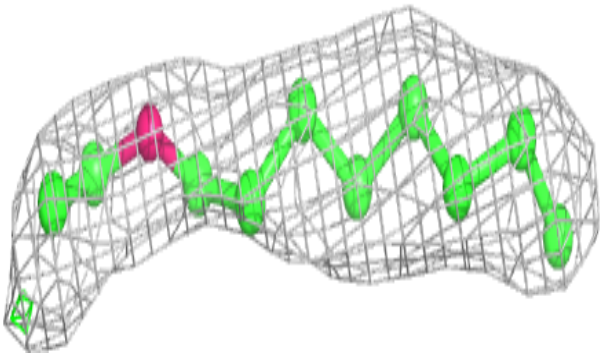
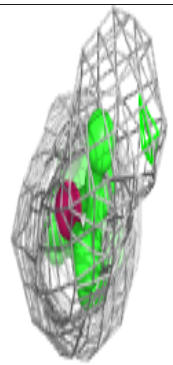
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around C8E C 1300:

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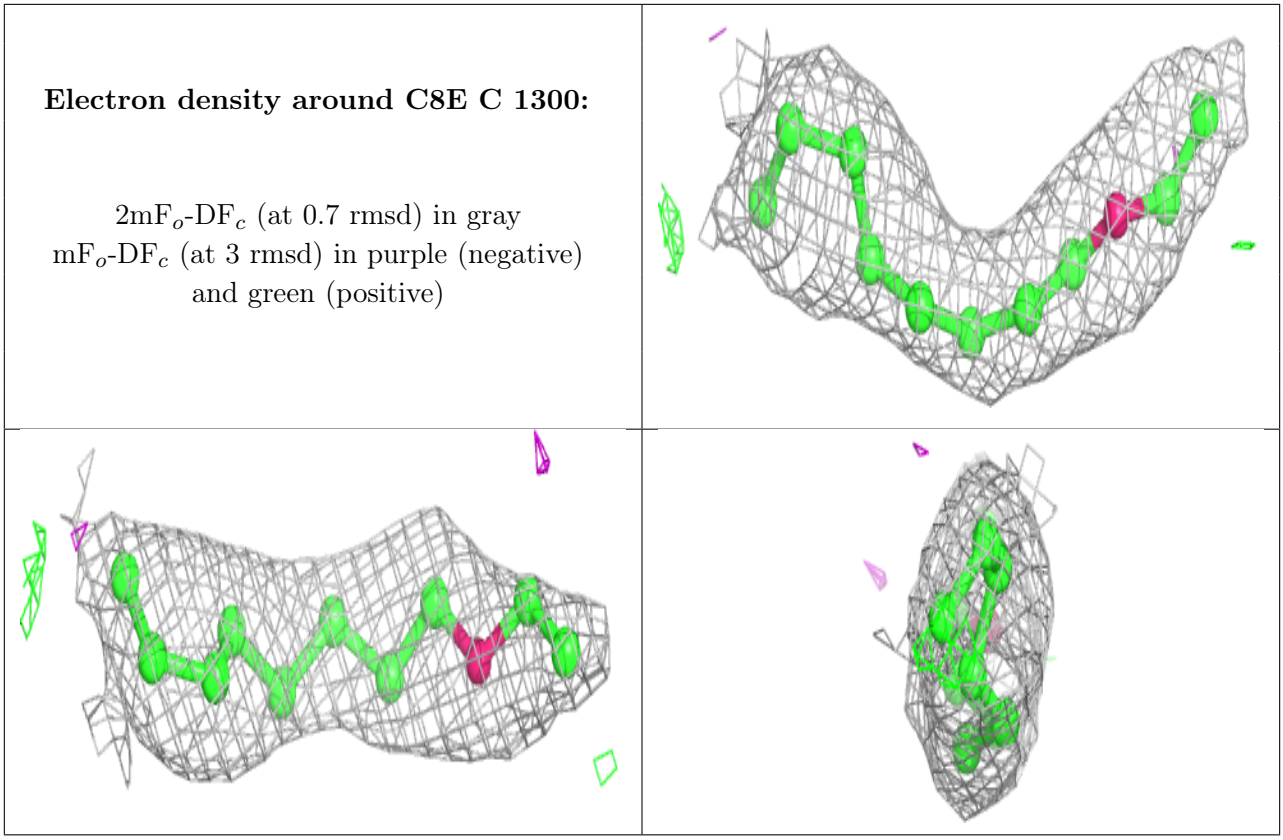
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C8E D 1302:

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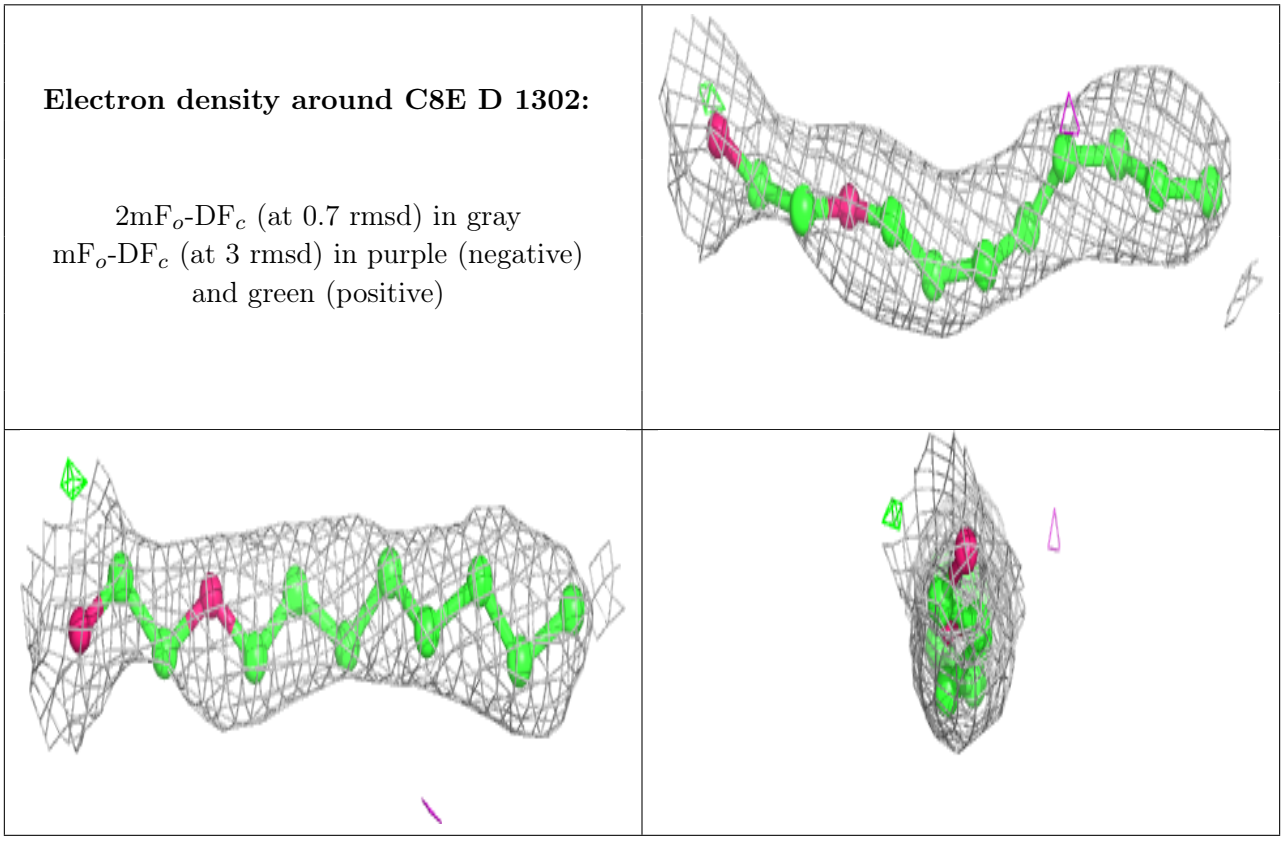
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C8E D 1304:

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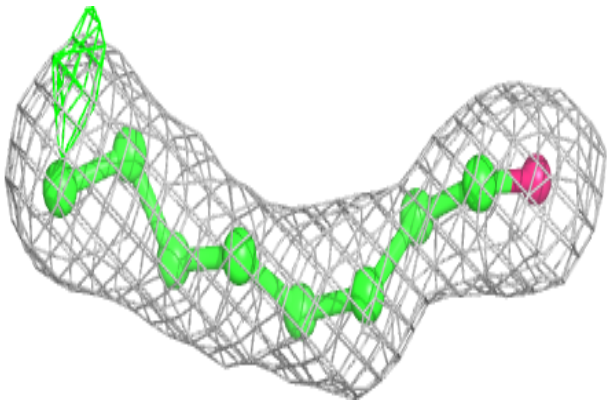
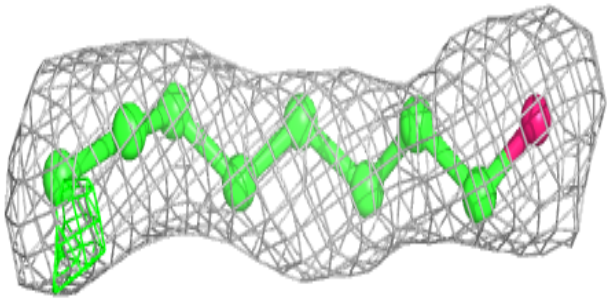
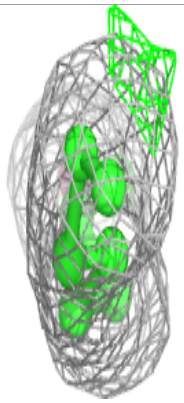
and green (positive)







Electron density around C8E C 1302:

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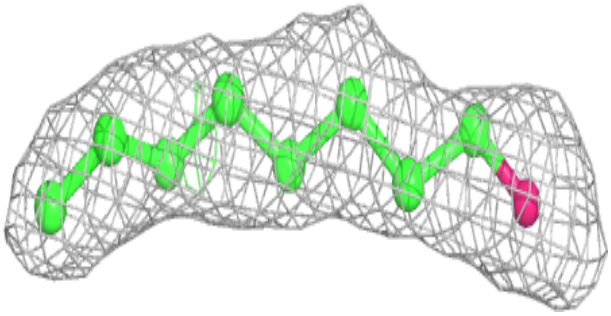
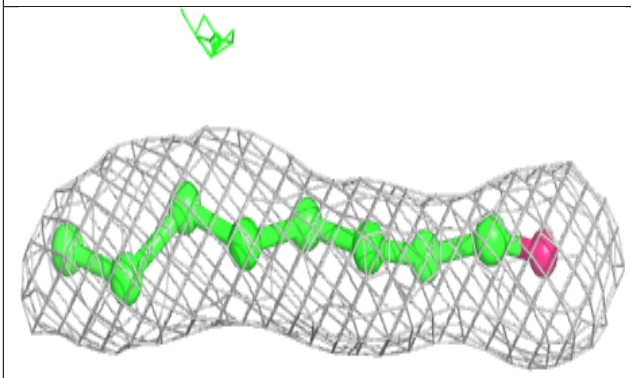
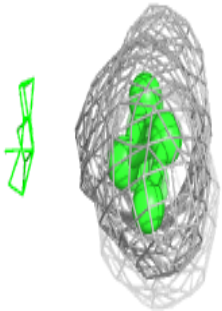
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around C8E A 1303:

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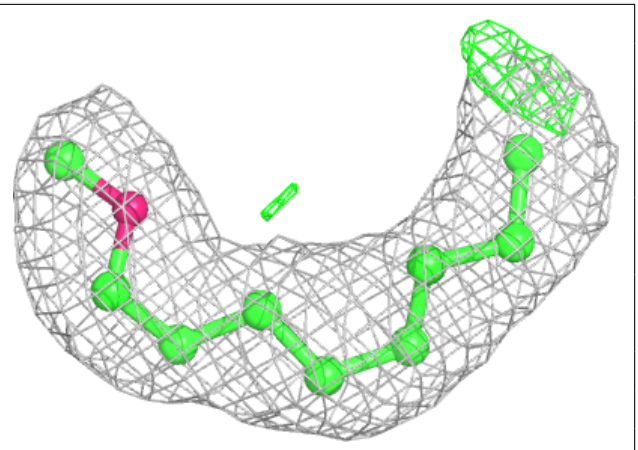
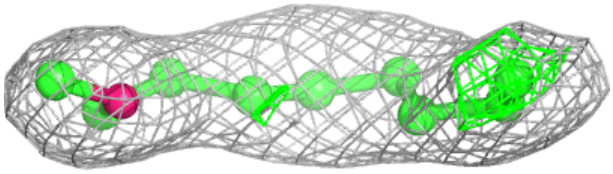
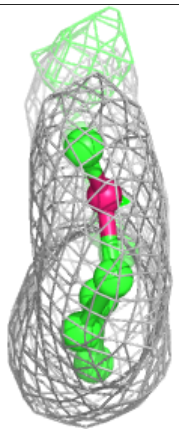
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around C8E D 1303:

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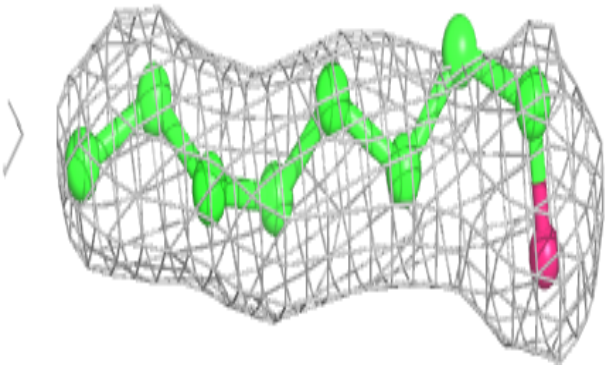
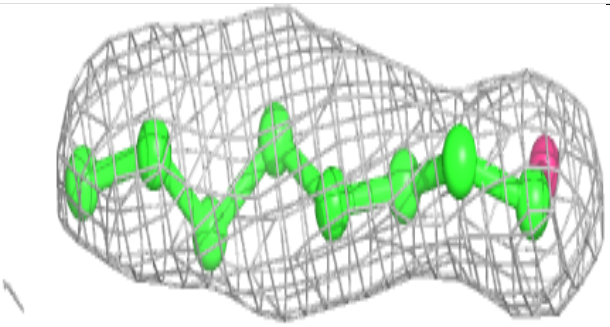
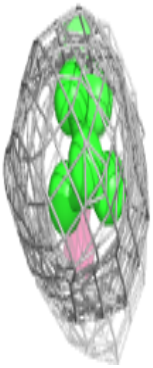
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around C8E B 1305:

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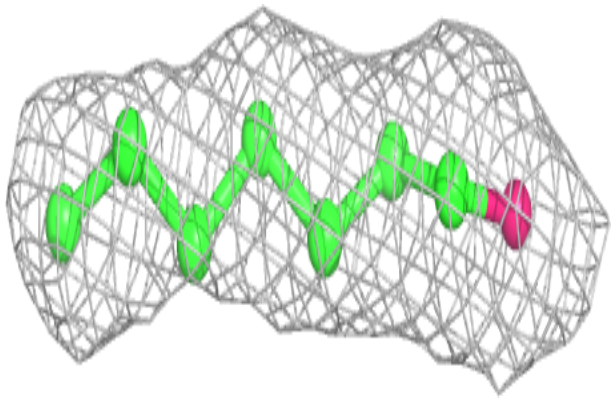
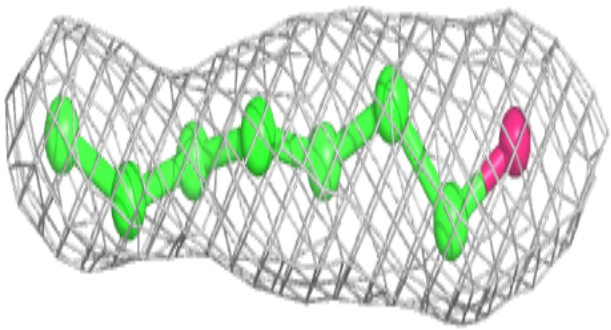
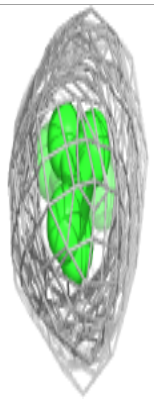
and green (positive)







Electron density around C8E B 1304:

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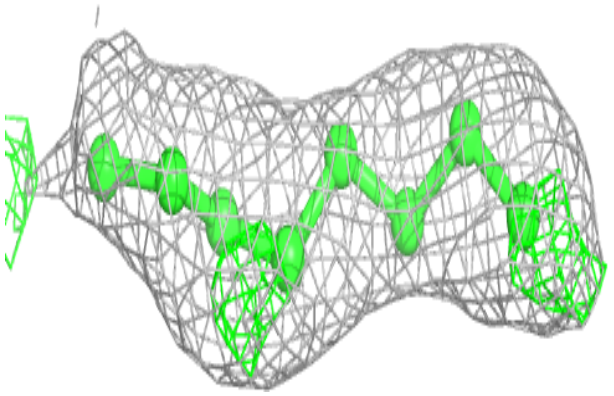
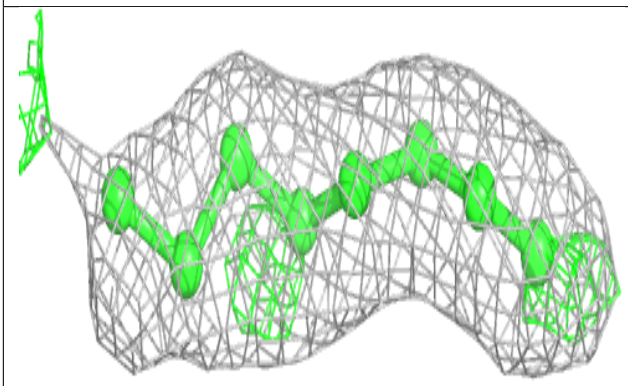
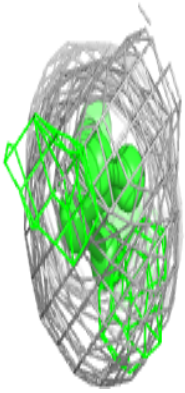
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

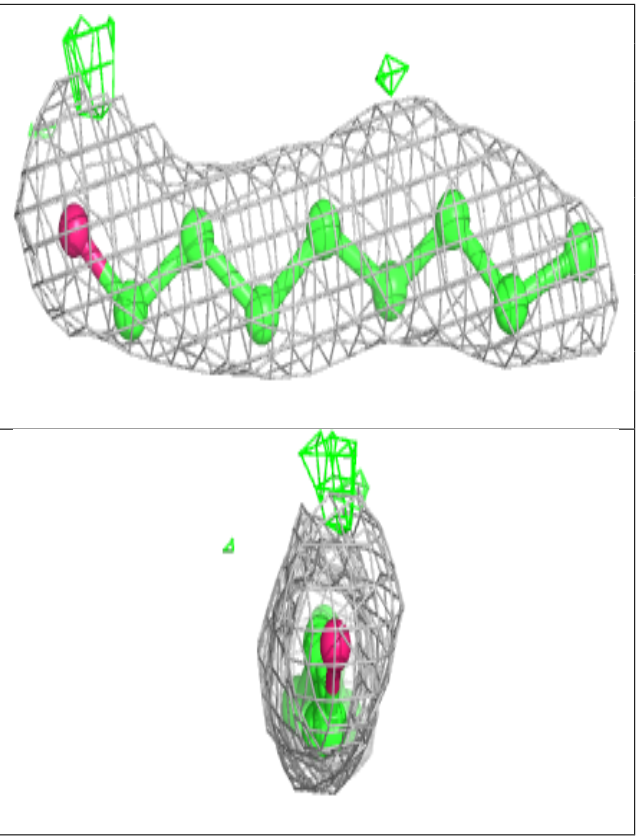






Electron density around C8E A 1301:

$2mF_o$-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 1302:

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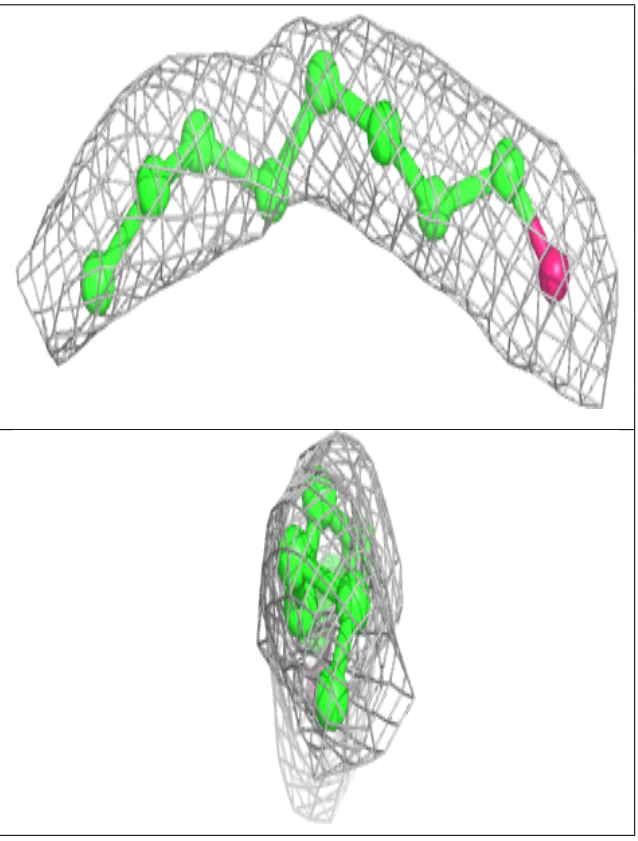
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C8E C 1301:

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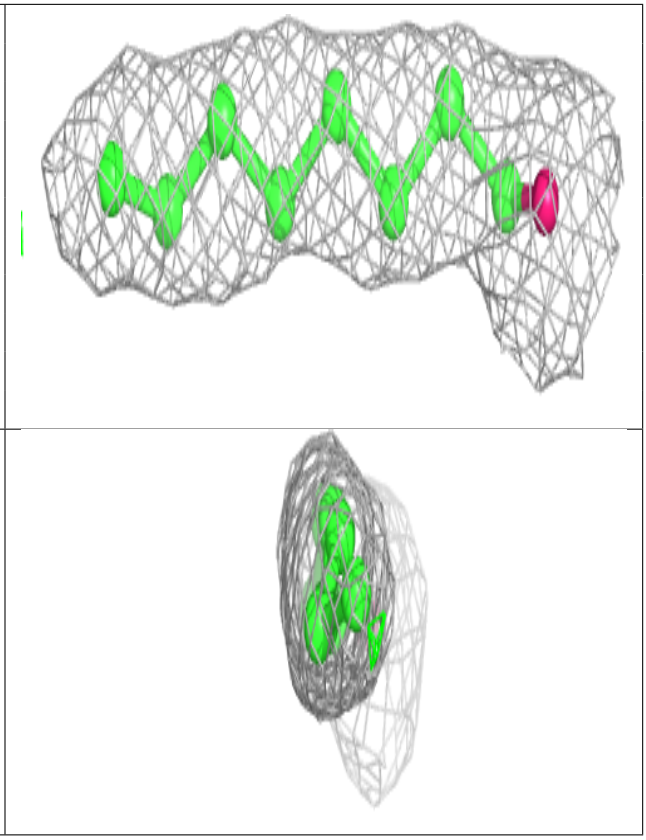
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.