Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 03:13 am BST

PDB ID	:	5NUQ
Title	:	Structural basis for maintenance of bacterial outer membrane lipid asymmetry
Authors	:	Abellon-Ruiz, J.; Kaptan, S.S.; Basle, A.; Claudi, B.; Bumann, D.; Kleinekathofer, U.; van den Berg, B.
Deposited on	:	2017-05-01
Resolution	:	3.20 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 following versions of software and data (see references (i)) were used in the production of this report:

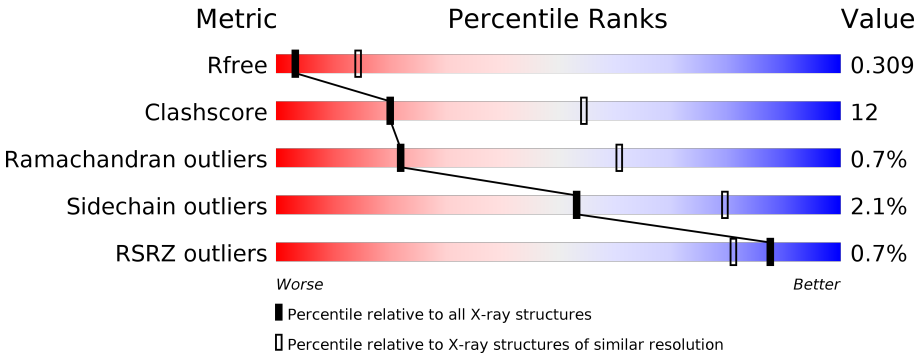
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	340	74% 25%
1	B	340	76% 24%
1	C	340	73% 26%
1	D	340	73% 26%
1	E	340	% 75% 24%
1	F	340	% 79% 20%

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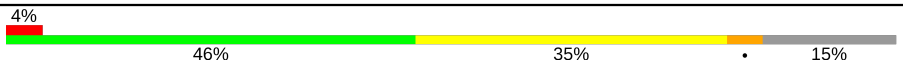
Mol	Chain	Length	Quality of chain
2	G	235	
2	H	235	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19044 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.

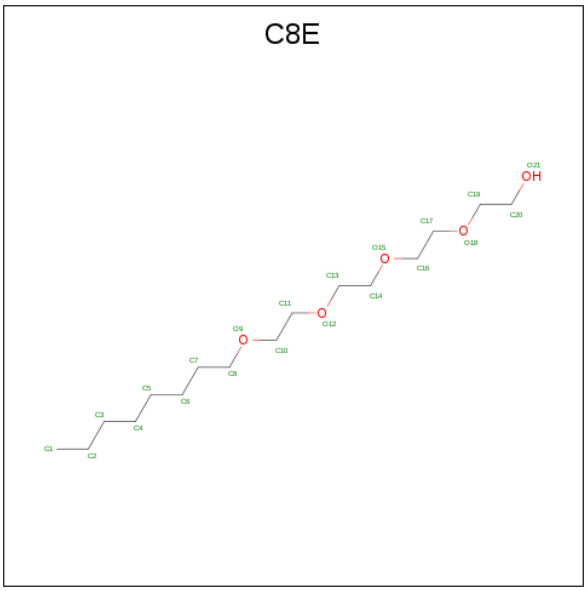
- Molecule 1 is a protein called Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	F	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

- Molecule 2 is a protein called Probable phospholipid-binding lipoprotein mlaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	200	Total	C	N	O	S	0	0	0
			1597	1026	269	292	10			
2	H	199	Total	C	N	O	S	0	0	0
			1593	1024	268	291	10			

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



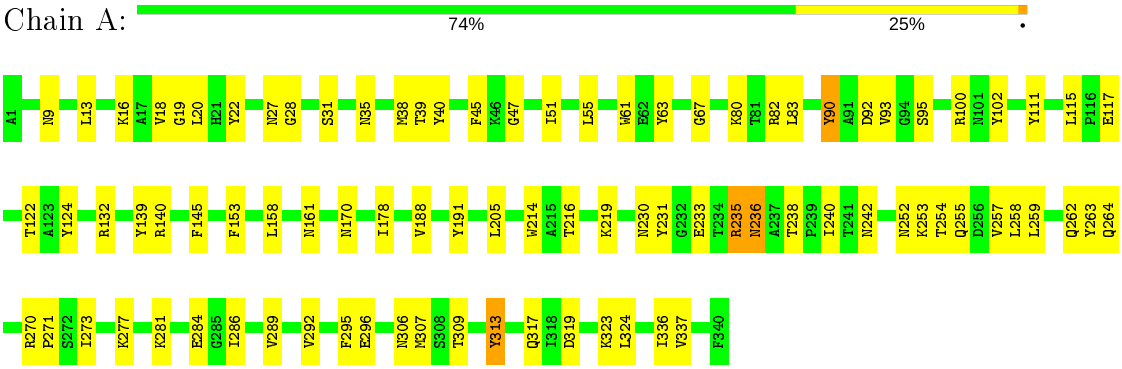
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 8 1	0	0
3	A	1	Total C O 12 10 2	0	0
3	B	1	Total C O 9 6 3	0	0
3	B	1	Total C O 9 8 1	0	0
3	D	1	Total C O 11 10 1	0	0
3	D	1	Total C O 9 8 1	0	0
3	F	1	Total C O 9 8 1	0	0
3	H	1	Total C O 11 9 2	0	0
3	H	1	Total C O 13 11 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

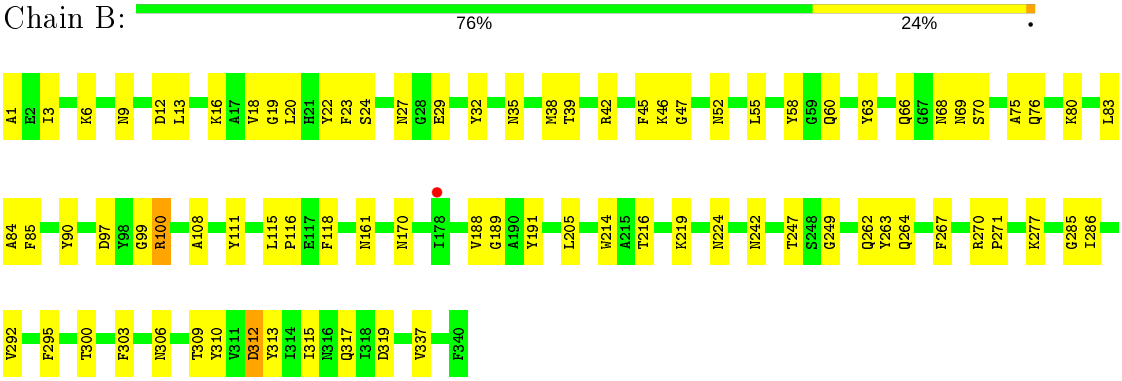
- Molecule 1: Outer membrane protein F

Chain A:



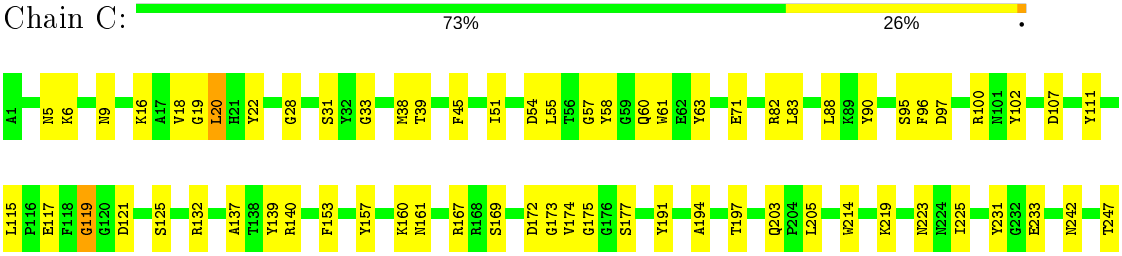
- Molecule 1: Outer membrane protein F

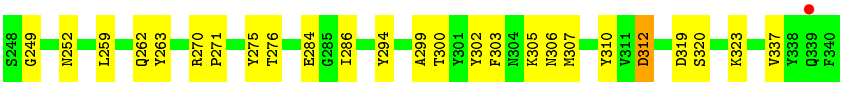
Chain B:



- Molecule 1: Outer membrane protein F

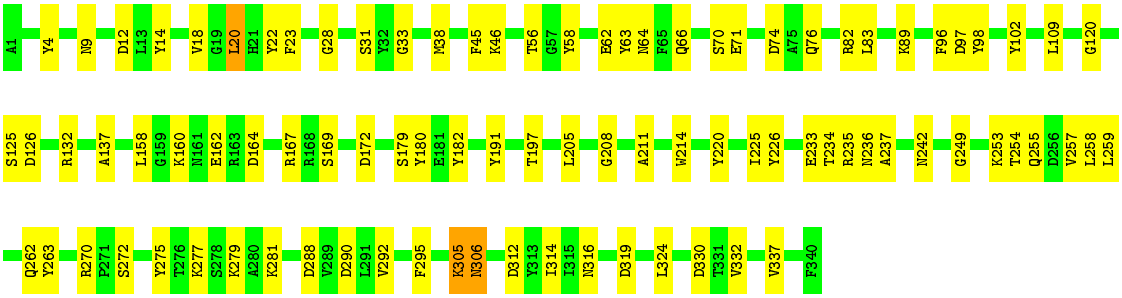
Chain C:





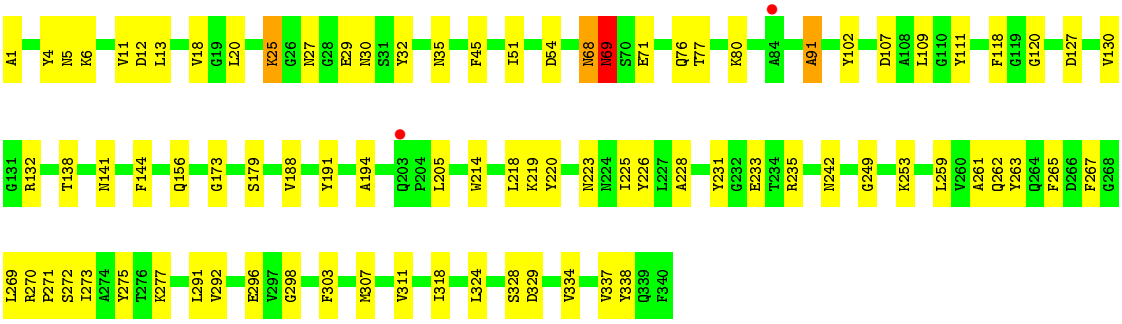
• Molecule 1: Outer membrane protein F

Chain D:



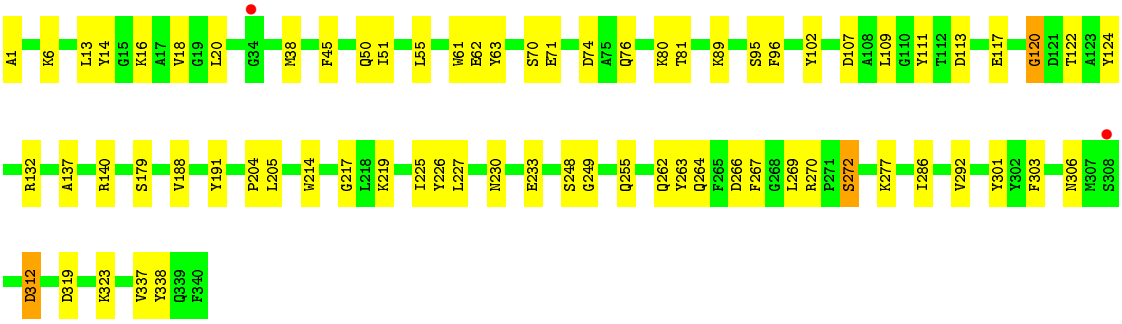
• Molecule 1: Outer membrane protein F

Chain E:



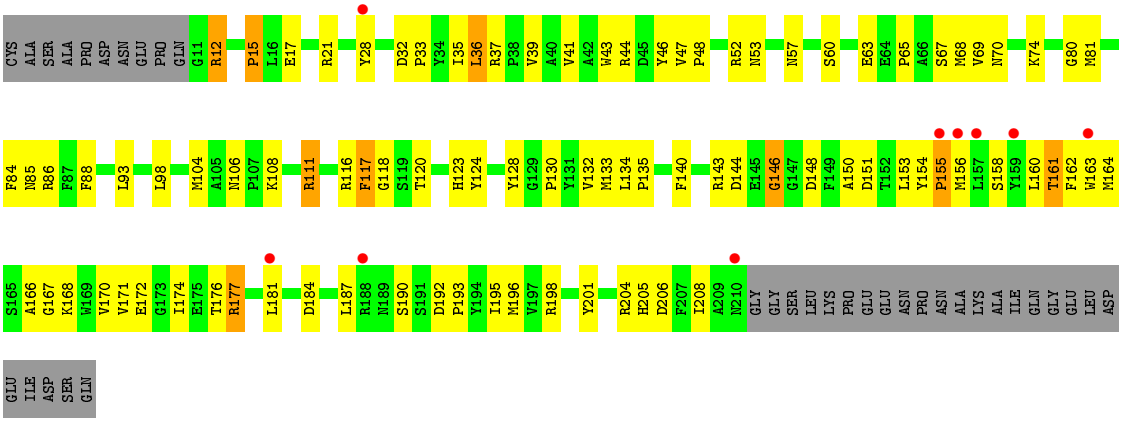
• Molecule 1: Outer membrane protein F

Chain F:



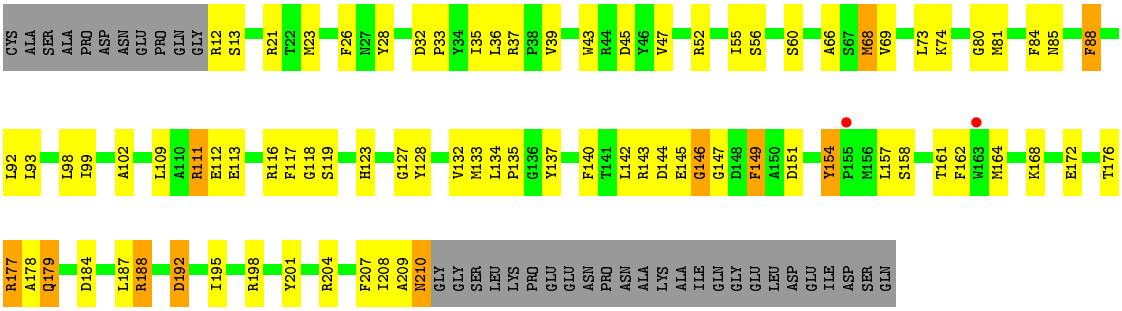
• Molecule 2: Probable phospholipid-binding lipoprotein mlaA

Chain G:



- Molecule 2: Probable phospholipid-binding lipoprotein mlaA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.49Å 163.04Å 230.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.24 – 3.20 94.24 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (94.24-3.20) 100.0 (94.24-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.238 , 0.306 0.243 , 0.309	Depositor DCC
R_{free} test set	5676 reflections (7.82%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	1.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	19044	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 40.85 % 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 2.5730e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.44	0/2683	0.90	4/3628 (0.1%)
1	B	0.42	0/2683	0.65	0/3628
1	C	0.43	0/2683	0.66	0/3628
1	D	0.44	0/2683	0.85	7/3628 (0.2%)
1	E	0.42	0/2683	0.69	2/3628 (0.1%)
1	F	0.41	0/2683	0.66	0/3628
2	G	0.42	0/1644	0.68	0/2231
2	H	0.48	0/1640	0.73	3/2226 (0.1%)
All	All	0.43	0/19382	0.74	16/26225 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	E	0	1
2	H	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	ASN	CB-CG-OD1	29.19	179.97	121.60
1	D	306	ASN	CB-CG-OD1	20.70	163.00	121.60
1	A	236	ASN	CB-CG-ND2	-17.12	75.60	116.70
1	D	306	ASN	CB-CG-ND2	-16.71	76.59	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	179	GLN	CG-CD-NE2	-11.16	89.91	116.70
1	D	306	ASN	N-CA-CB	-10.66	91.41	110.60
1	A	236	ASN	OD1-CG-ND2	-7.61	104.39	121.90
1	E	68	ASN	C-N-CA	-7.49	102.97	121.70
1	D	306	ASN	OD1-CG-ND2	-7.29	105.14	121.90
1	A	235	ARG	C-N-CA	7.08	139.40	121.70
2	H	179	GLN	CG-CD-OE1	6.94	135.48	121.60
1	D	305	LYS	C-N-CA	6.86	138.84	121.70
1	D	306	ASN	CB-CA-C	6.20	122.80	110.40
2	H	178	ALA	C-N-CA	-6.05	106.58	121.70
1	D	306	ASN	N-CA-C	5.26	125.20	111.00
1	E	69	ASN	CB-CG-ND2	-5.01	104.67	116.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ASN	Mainchain
1	D	305	LYS	Peptide
1	D	306	ASN	Sidechain
1	E	69	ASN	Sidechain
2	H	179	GLN	Sidechain

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	2627	0	2444	64	0
1	B	2627	0	2444	63	0
1	C	2627	0	2444	57	0
1	D	2627	0	2444	63	0
1	E	2627	0	2444	65	0
1	F	2627	0	2444	46	0
2	G	1597	0	1522	67	0
2	H	1593	0	1519	70	0
3	A	21	0	33	4	0
3	B	18	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	20	0	31	4	0
3	F	9	0	17	0	0
3	H	24	0	37	3	0
All	All	19044	0	17846	460	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 12.

All (460) 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)
2:G:60:SER:OG	2:G:111:ARG:NH1	2.02	0.93
2:H:21:ARG:NH1	2:H:192:ASP:OD1	2.03	0.91
1:C:20:LEU:HD23	1:C:38:MET:HB2	1.54	0.88
1:C:203:GLN:HG2	1:C:249:GLY:HA2	1.57	0.87
1:D:20:LEU:HD23	1:D:38:MET:HB2	1.58	0.86
1:D:262:GLN:OE1	1:D:270:ARG:NH1	2.10	0.85
1:F:117:GLU:N	1:F:312:ASP:OD2	2.12	0.83
1:F:262:GLN:HG2	1:F:272:SER:HB2	1.59	0.81
1:F:262:GLN:OE1	1:F:270:ARG:NH1	2.14	0.80
1:C:262:GLN:OE1	1:C:270:ARG:NH1	2.15	0.80
2:G:37:ARG:HG2	2:G:177:ARG:HH12	1.47	0.79
1:B:262:GLN:OE1	1:B:270:ARG:NH1	2.15	0.79
1:B:76:GLN:NE2	1:D:63:TYR:OH	2.13	0.79
2:G:154:TYR:HB2	2:G:155:PRO:HD2	1.65	0.78
1:D:180:TYR:HE2	1:D:182:TYR:HB2	1.51	0.75
2:G:35:ILE:O	2:G:36:LEU:HB2	1.86	0.75
1:A:235:ARG:HD3	1:A:253:LYS:HG3	1.69	0.75
1:E:68:ASN:C	1:E:69:ASN:HD22	1.91	0.74
1:A:262:GLN:OE1	1:A:270:ARG:NH1	2.20	0.74
1:E:233:GLU:HB3	1:E:235:ARG:HH12	1.51	0.74
2:H:209:ALA:O	2:H:210:ASN:ND2	2.21	0.73
1:E:242:ASN:HB2	1:E:324:LEU:CD2	2.18	0.73
1:F:111:TYR:O	1:F:226:TYR:OH	2.07	0.73
1:B:242:ASN:HB3	1:B:247:THR:HG22	1.70	0.72
2:H:32:ASP:HA	2:H:36:LEU:HB2	1.69	0.72
2:G:15:PRO:HG2	2:G:130:PRO:HB3	1.71	0.72
1:A:313:TYR:CZ	1:B:315:ILE:HG21	2.25	0.72
1:E:242:ASN:HB2	1:E:324:LEU:HD22	1.71	0.72
1:E:262:GLN:OE1	1:E:270:ARG:NH1	2.22	0.70
2:H:28:TYR:OH	2:H:188:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:SER:HB2	1:E:188:VAL:HG12	1.73	0.70
1:C:242:ASN:HB3	1:C:247:THR:HG22	1.74	0.69
1:A:16:LYS:HE3	1:A:18:VAL:HG21	1.75	0.69
1:A:22:TYR:OH	1:A:117:GLU:OE2	2.08	0.68
1:D:242:ASN:HD22	1:D:324:LEU:HD23	1.59	0.68
2:H:28:TYR:OH	2:H:187:LEU:HB3	1.93	0.68
2:G:69:VAL:HG21	2:G:154:TYR:CE2	2.30	0.67
2:G:65:PRO:HG2	2:G:156:MET:HB2	1.77	0.67
1:A:93:VAL:HG11	2:H:99:ILE:HG23	1.77	0.67
1:E:18:VAL:HG22	1:E:337:VAL:HG22	1.75	0.67
1:D:205:LEU:HB2	1:D:249:GLY:HA3	1.77	0.66
1:E:259:LEU:HD12	1:E:275:TYR:HD2	1.60	0.66
1:C:125:SER:O	1:C:167:ARG:NH2	2.23	0.66
2:G:12:ARG:NH1	2:G:17:GLU:OE1	2.24	0.66
2:H:127:GLY:H	2:H:143:ARG:HH11	1.44	0.66
1:B:16:LYS:HE3	1:B:18:VAL:HG21	1.75	0.66
2:H:161:THR:HG23	2:H:164:MET:H	1.61	0.65
1:C:169:SER:HB3	1:C:197:THR:HG21	1.77	0.65
1:D:56:THR:HG22	1:D:89:LYS:HB3	1.79	0.65
2:G:12:ARG:HD2	2:G:198:ARG:HH22	1.60	0.65
1:E:235:ARG:HD3	1:E:253:LYS:HG2	1.79	0.65
2:H:85:ASN:HD21	2:H:109:LEU:HD21	1.59	0.64
2:G:53:ASN:O	2:G:57:ASN:ND2	2.31	0.64
1:D:214:TRP:CZ2	1:D:233:GLU:HB2	2.32	0.64
1:C:19:GLY:HA2	1:C:39:THR:HG23	1.80	0.63
1:F:18:VAL:HG22	1:F:337:VAL:HG22	1.79	0.63
2:H:74:LYS:HA	2:H:123:HIS:HD2	1.64	0.63
1:A:63:TYR:OH	1:E:76:GLN:NE2	2.32	0.63
1:B:303:PHE:HE2	1:B:309:THR:HG23	1.62	0.63
1:A:51:ILE:HB	1:A:55:LEU:HB3	1.81	0.63
1:B:9:ASN:ND2	1:F:306:ASN:OD1	2.31	0.63
2:G:177:ARG:NH2	2:G:184:ASP:OD2	2.32	0.62
2:G:68:MET:HG3	2:G:80:GLY:O	1.99	0.62
2:G:28:TYR:CZ	2:G:187:LEU:HD12	2.34	0.62
1:C:303:PHE:HB3	1:E:51:ILE:HG12	1.80	0.62
1:E:191:TYR:HD1	1:E:214:TRP:HB3	1.64	0.62
1:B:115:LEU:HD12	1:B:118:PHE:O	2.00	0.62
1:E:111:TYR:CE1	1:E:219:LYS:HD3	2.34	0.62
1:D:235:ARG:HE	1:D:253:LYS:HD3	1.64	0.62
2:H:74:LYS:HZ1	2:H:119:SER:HB2	1.65	0.62
1:A:47:GLY:HA3	1:E:338:TYR:CE2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:ARG:HB3	2:G:151:ASP:OD2	2.00	0.62
1:C:102:TYR:CE1	1:C:132:ARG:HG3	2.34	0.61
1:A:45:PHE:CE2	1:A:61:TRP:HB3	2.35	0.61
1:C:45:PHE:CE2	1:C:61:TRP:HB3	2.35	0.61
1:D:225:ILE:HG12	1:D:263:TYR:HD1	1.66	0.61
1:C:300:THR:HG23	1:C:310:TYR:HB3	1.82	0.61
1:E:27:ASN:O	1:E:35:ASN:HB3	2.00	0.61
2:H:192:ASP:HB3	2:H:195:ILE:HB	1.82	0.61
1:E:25:LYS:HE2	1:E:329:ASP:OD2	2.00	0.61
1:F:96:PHE:CE1	1:F:137:ALA:HB1	2.35	0.61
1:D:64:ASN:ND2	1:D:66:GLN:OE1	2.33	0.61
2:H:66:ALA:HA	2:H:154:TYR:HE1	1.66	0.60
1:D:98:TYR:CE1	3:D:402:C8E:H71	2.37	0.60
1:A:255:GLN:OE1	1:A:281:LYS:NZ	2.28	0.60
2:H:37:ARG:HD2	2:H:177:ARG:HH12	1.67	0.59
1:A:19:GLY:HA2	1:A:39:THR:HG23	1.83	0.59
1:C:231:TYR:OH	1:C:233:GLU:OE2	2.18	0.59
1:D:70:SER:OG	1:D:74:ASP:OD1	2.16	0.59
2:G:128:TYR:HA	2:G:143:ARG:HB3	1.83	0.59
1:E:4:TYR:HD2	1:E:11:VAL:HG23	1.68	0.59
1:D:71:GLU:HB3	1:F:80:LYS:HD2	1.84	0.59
1:F:14:TYR:OH	1:F:62:GLU:OE1	2.16	0.59
1:B:90:TYR:OH	2:G:93:LEU:O	2.16	0.58
1:B:66:GLN:NE2	1:B:68:ASN:OD1	2.37	0.58
1:A:158:LEU:HD21	1:A:170:ASN:HD22	1.68	0.58
1:B:319:ASP:N	1:B:319:ASP:OD1	2.36	0.58
2:G:118:GLY:HA3	2:G:144:ASP:HA	1.86	0.58
1:C:121:ASP:OD1	1:C:294:TYR:OH	2.14	0.58
1:C:191:TYR:HD1	1:C:214:TRP:HB3	1.68	0.58
2:G:69:VAL:HG21	2:G:154:TYR:CZ	2.39	0.58
1:E:68:ASN:C	1:E:69:ASN:ND2	2.58	0.57
2:H:12:ARG:HB2	2:H:198:ARG:HH22	1.69	0.57
1:D:169:SER:HB3	1:D:197:THR:HG21	1.86	0.57
1:D:211:ALA:HB1	1:D:237:ALA:HB2	1.85	0.57
1:A:102:TYR:CE1	1:A:132:ARG:HG3	2.39	0.57
1:E:233:GLU:OE1	1:E:235:ARG:NH2	2.28	0.57
1:E:291:LEU:HD21	1:E:324:LEU:HD12	1.87	0.57
2:G:151:ASP:HA	2:G:154:TYR:CE1	2.39	0.57
2:H:151:ASP:HA	2:H:154:TYR:CD2	2.40	0.57
2:H:56:SER:HB3	2:H:111:ARG:HH22	1.70	0.57
2:G:160:LEU:O	2:G:164:MET:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:65:PRO:HG2	2:G:156:MET:CB	2.35	0.57
1:B:18:VAL:O	1:B:39:THR:OG1	2.20	0.57
1:C:319:ASP:OD1	1:C:319:ASP:N	2.37	0.56
2:G:37:ARG:HG2	2:G:177:ARG:NH1	2.19	0.56
1:C:117:GLU:N	1:C:312:ASP:OD2	2.38	0.56
1:C:28:GLY:O	1:C:31:SER:OG	2.24	0.56
1:D:316:ASN:H	1:D:330:ASP:HB3	1.71	0.56
2:H:69:VAL:HG11	2:H:154:TYR:CE1	2.41	0.56
1:F:102:TYR:CE1	1:F:132:ARG:HG3	2.40	0.56
1:D:255:GLN:OE1	1:D:281:LYS:NZ	2.38	0.56
1:D:180:TYR:CE2	1:D:182:TYR:HB2	2.37	0.56
1:E:277:LYS:HA	1:E:292:VAL:O	2.06	0.56
1:F:319:ASP:OD1	1:F:319:ASP:N	2.37	0.56
1:D:160:LYS:NZ	1:D:162:GLU:OE1	2.34	0.55
1:F:191:TYR:HD1	1:F:214:TRP:HB3	1.71	0.55
1:B:76:GLN:HE22	1:D:63:TYR:HH	1.47	0.55
1:F:286:ILE:HG23	1:F:323:LYS:HD2	1.88	0.55
2:H:154:TYR:O	2:H:158:SER:OG	2.18	0.55
2:H:12:ARG:HB2	2:H:198:ARG:NH2	2.21	0.55
1:B:108:ALA:HA	1:B:188:VAL:HG11	1.87	0.55
2:G:172:GLU:O	2:G:176:THR:OG1	2.24	0.55
1:B:38:MET:C	1:B:68:ASN:HD21	2.10	0.55
2:G:116:ARG:NH1	2:G:148:ASP:O	2.40	0.54
2:G:161:THR:OG1	2:G:162:PHE:N	2.40	0.54
2:H:66:ALA:HA	2:H:154:TYR:CE1	2.42	0.54
2:G:192:ASP:HB3	2:G:195:ILE:HB	1.89	0.54
1:B:32:TYR:HE2	1:B:118:PHE:CD1	2.25	0.54
1:D:125:SER:O	1:D:167:ARG:NH2	2.33	0.54
2:H:146:GLY:O	2:H:149:PHE:HB3	2.07	0.54
2:H:204:ARG:O	2:H:208:ILE:HG12	2.07	0.54
2:H:43:TRP:O	2:H:47:VAL:HG22	2.06	0.54
2:H:74:LYS:HA	2:H:123:HIS:CD2	2.42	0.54
1:B:224:ASN:ND2	1:B:264:GLN:O	2.41	0.54
1:E:179:SER:HB2	1:E:188:VAL:CG1	2.36	0.54
2:H:102:ALA:HB1	2:H:109:LEU:HD23	1.90	0.53
1:C:111:TYR:CE1	1:C:219:LYS:HD3	2.42	0.53
1:A:93:VAL:O	1:A:139:TYR:OH	2.25	0.53
1:F:277:LYS:HA	1:F:292:VAL:O	2.09	0.53
1:B:263:TYR:O	1:B:271:PRO:HD2	2.09	0.53
1:A:90:TYR:OH	2:H:93:LEU:O	2.24	0.53
1:C:205:LEU:HA	1:C:284:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ASN:N	1:E:69:ASN:ND2	2.57	0.53
1:F:70:SER:OG	1:F:74:ASP:OD1	2.25	0.53
1:A:13:LEU:HD22	1:E:13:LEU:HD21	1.89	0.53
1:C:300:THR:HB	1:C:302:TYR:HE2	1.74	0.53
1:D:96:PHE:HE1	1:D:137:ALA:HB1	1.73	0.53
1:E:269:LEU:HD22	2:H:85:ASN:HB3	1.91	0.53
1:C:18:VAL:HG22	1:C:337:VAL:HG22	1.91	0.53
1:F:264:GLN:OE1	1:F:270:ARG:HB2	2.09	0.52
1:B:295:PHE:HD2	1:B:317:GLN:NE2	2.06	0.52
1:C:71:GLU:HB3	1:E:80:LYS:HD2	1.92	0.52
1:F:51:ILE:HG21	1:F:55:LEU:HD23	1.91	0.52
1:A:16:LYS:HE3	1:A:18:VAL:CG2	2.38	0.52
1:E:32:TYR:HE2	1:E:118:PHE:CD1	2.27	0.52
2:G:154:TYR:O	2:G:158:SER:OG	2.19	0.52
1:D:319:ASP:N	1:D:319:ASP:OD1	2.35	0.52
2:G:43:TRP:O	2:G:47:VAL:HG12	2.10	0.52
1:D:259:LEU:HD12	1:D:275:TYR:HD2	1.74	0.52
2:H:127:GLY:C	2:H:143:ARG:HD3	2.30	0.52
2:H:128:TYR:HA	2:H:143:ARG:HB3	1.92	0.52
1:D:12:ASP:HB3	1:D:46:LYS:HB2	1.92	0.51
1:E:29:GLU:HG3	1:E:30:ASN:N	2.24	0.51
1:A:277:LYS:HA	1:A:292:VAL:O	2.10	0.51
1:B:191:TYR:HD1	1:B:214:TRP:HB3	1.75	0.51
2:H:37:ARG:CD	2:H:177:ARG:HH12	2.23	0.51
1:F:205:LEU:HB2	1:F:249:GLY:HA3	1.93	0.51
1:A:122:THR:HA	1:A:124:TYR:CE1	2.45	0.51
1:D:262:GLN:HE21	1:D:272:SER:HB2	1.76	0.51
1:A:27:ASN:O	1:A:35:ASN:HB3	2.11	0.51
2:H:117:PHE:HB3	2:H:147:GLY:O	2.11	0.51
1:E:1:ALA:N	1:E:13:LEU:O	2.39	0.51
1:B:47:GLY:HA3	1:F:338:TYR:CE2	2.47	0.50
2:H:99:ILE:CD1	3:H:302:C8E:H21	2.42	0.50
1:A:205:LEU:HB3	1:A:240:ILE:HD11	1.92	0.50
1:F:111:TYR:CE2	1:F:188:VAL:HG12	2.46	0.50
2:G:204:ARG:O	2:G:208:ILE:HG12	2.11	0.50
1:A:158:LEU:HD11	1:A:170:ASN:HD21	1.76	0.50
1:B:111:TYR:CE1	1:B:219:LYS:HD3	2.46	0.50
1:E:141:ASN:OD1	1:E:144:PHE:HA	2.11	0.50
2:H:177:ARG:NH2	2:H:184:ASP:OD1	2.45	0.50
1:A:92:ASP:O	1:A:145:PHE:HA	2.12	0.50
1:D:102:TYR:CE1	1:D:132:ARG:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:106:ASN:HD21	2:G:108:LYS:HB2	1.76	0.50
1:A:319:ASP:N	1:A:319:ASP:OD1	2.45	0.50
1:A:295:PHE:HD1	1:A:317:GLN:NE2	2.09	0.50
2:G:144:ASP:OD2	2:G:205:HIS:ND1	2.38	0.50
1:B:1:ALA:HB1	1:D:4:TYR:CE1	2.47	0.50
1:B:277:LYS:HA	1:B:292:VAL:O	2.11	0.50
1:F:16:LYS:HE3	1:F:18:VAL:HG21	1.94	0.50
2:H:60:SER:OG	2:H:111:ARG:NH1	2.43	0.49
1:A:264:GLN:OE1	1:A:270:ARG:HB2	2.12	0.49
1:D:214:TRP:CE2	1:D:233:GLU:HB2	2.47	0.49
2:H:32:ASP:HB3	2:H:33:PRO:HD3	1.94	0.49
1:C:205:LEU:HB2	1:C:249:GLY:HA3	1.94	0.49
2:G:32:ASP:HB3	2:G:33:PRO:HD3	1.94	0.49
2:H:35:ILE:O	2:H:39:VAL:HG23	2.12	0.49
1:A:259:LEU:HD22	3:A:402:C8E:H71	1.93	0.49
1:C:263:TYR:O	1:C:271:PRO:HD2	2.12	0.49
1:D:191:TYR:HD1	1:D:214:TRP:HB3	1.76	0.49
2:G:154:TYR:N	2:G:158:SER:OG	2.45	0.49
1:D:257:VAL:O	1:D:258:LEU:HD12	2.11	0.49
1:D:56:THR:CG2	1:D:89:LYS:HB3	2.42	0.49
1:F:111:TYR:CE1	1:F:219:LYS:HD3	2.48	0.49
1:D:76:GLN:NE2	1:F:63:TYR:OH	2.37	0.49
1:B:18:VAL:HG22	1:B:337:VAL:HG22	1.93	0.49
1:C:259:LEU:HD12	1:C:275:TYR:HD2	1.78	0.49
3:A:401:C8E:H51	1:B:267:PHE:HE2	1.77	0.49
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.48	0.49
2:H:81:MET:HA	2:H:84:PHE:HB3	1.95	0.49
1:B:39:THR:N	1:B:68:ASN:HD21	2.10	0.49
1:B:52:ASN:OD1	1:B:55:LEU:N	2.42	0.49
1:D:62:GLU:HG2	1:D:82:ARG:HG3	1.95	0.49
1:B:19:GLY:HA2	1:B:39:THR:OG1	2.12	0.48
2:H:118:GLY:HA3	2:H:144:ASP:HA	1.94	0.48
1:C:173:GLY:HA3	1:C:194:ALA:HB2	1.95	0.48
1:B:111:TYR:CE2	1:B:188:VAL:HG12	2.48	0.48
1:C:57:GLY:HA2	1:C:88:LEU:HD23	1.96	0.48
1:C:58:TYR:OH	1:C:97:ASP:HB3	2.13	0.48
1:D:20:LEU:HD21	1:D:22:TYR:CE1	2.48	0.48
1:E:311:VAL:HG23	2:H:88:PHE:CE1	2.49	0.48
2:H:142:LEU:HD23	2:H:142:LEU:O	2.12	0.48
1:B:23:PHE:HZ	3:D:402:C8E:H61	1.78	0.48
1:C:252:ASN:ND2	1:C:284:GLU:OE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:ASP:O	2:H:146:GLY:N	2.43	0.48
2:H:161:THR:OG1	2:H:162:PHE:N	2.46	0.48
1:D:28:GLY:O	1:D:31:SER:OG	2.29	0.48
1:E:318:ILE:HB	1:E:328:SER:HA	1.95	0.48
1:A:306:ASN:OD1	1:C:9:ASN:ND2	2.47	0.48
1:D:172:ASP:N	1:D:172:ASP:OD2	2.39	0.48
1:F:269:LEU:HB2	2:G:85:ASN:ND2	2.29	0.48
2:H:151:ASP:O	2:H:157:LEU:HB2	2.13	0.48
2:G:144:ASP:O	2:G:146:GLY:N	2.43	0.48
1:A:216:THR:O	1:A:230:ASN:ND2	2.41	0.48
2:G:47:VAL:HG22	2:G:48:PRO:HD2	1.95	0.48
2:G:12:ARG:CD	2:G:198:ARG:HH22	2.26	0.47
2:H:98:LEU:HB3	3:H:302:C8E:H22	1.96	0.47
1:D:96:PHE:CE1	1:D:137:ALA:HB1	2.49	0.47
2:H:112:GLU:OE2	2:H:113:GLU:HG2	2.14	0.47
1:C:16:LYS:HE3	1:C:18:VAL:HG21	1.97	0.47
1:E:54:ASP:HB3	1:E:91:ALA:HB2	1.95	0.47
1:F:267:PHE:HE1	2:G:85:ASN:HD22	1.62	0.47
1:B:83:LEU:HD13	1:B:85:PHE:HE2	1.79	0.47
1:E:205:LEU:HB2	1:E:249:GLY:HA3	1.96	0.47
1:E:291:LEU:CD2	1:E:324:LEU:HD12	2.45	0.47
1:D:82:ARG:O	1:D:83:LEU:HD23	2.14	0.47
1:D:220:TYR:O	1:D:226:TYR:HA	2.13	0.47
2:H:127:GLY:N	2:H:143:ARG:HH11	2.10	0.47
1:E:231:TYR:OH	1:E:233:GLU:OE2	2.30	0.47
1:B:111:TYR:CD1	1:B:219:LYS:HD3	2.50	0.47
1:B:300:THR:HG23	1:B:310:TYR:HB3	1.96	0.47
2:G:128:TYR:OH	2:G:206:ASP:OD1	2.22	0.47
2:G:39:VAL:O	2:G:43:TRP:N	2.48	0.47
1:D:22:TYR:HD2	1:D:33:GLY:O	1.98	0.46
2:H:145:GLU:OE1	2:H:201:TYR:OH	2.33	0.46
1:A:158:LEU:HD11	1:A:170:ASN:ND2	2.30	0.46
1:E:272:SER:N	1:E:298:GLY:O	2.44	0.46
1:E:263:TYR:O	1:E:271:PRO:HD2	2.16	0.46
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.81	0.46
2:G:187:LEU:HD13	2:G:193:PRO:HB3	1.97	0.46
2:G:81:MET:HA	2:G:84:PHE:HB3	1.97	0.46
1:A:216:THR:N	1:A:231:TYR:O	2.41	0.46
1:A:111:TYR:CE2	1:A:188:VAL:HG12	2.51	0.46
1:C:271:PRO:HA	1:C:299:ALA:HB2	1.98	0.46
2:G:65:PRO:O	2:G:69:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:116:ARG:HB3	2:H:151:ASP:OD2	2.15	0.46
1:C:107:ASP:OD2	1:C:140:ARG:NH1	2.49	0.45
1:B:70:SER:HB2	1:D:126:ASP:OD2	2.16	0.45
2:G:81:MET:O	2:G:85:ASN:N	2.38	0.45
2:H:168:LYS:O	2:H:172:GLU:HG3	2.17	0.45
2:G:150:ALA:O	2:G:153:LEU:HD12	2.16	0.45
2:G:168:LYS:O	2:G:172:GLU:HG3	2.15	0.45
2:G:21:ARG:HH12	2:G:192:ASP:CG	2.19	0.45
1:B:161:ASN:HB2	1:B:170:ASN:OD1	2.17	0.45
1:C:161:ASN:O	1:C:169:SER:HA	2.17	0.45
1:E:12:ASP:O	1:E:45:PHE:HA	2.16	0.45
1:F:6:LYS:HA	1:F:6:LYS:HD3	1.67	0.45
1:A:18:VAL:O	1:A:39:THR:HG23	2.17	0.45
1:D:18:VAL:HG22	1:D:337:VAL:HG22	1.99	0.45
1:B:1:ALA:HB1	1:D:4:TYR:CD1	2.52	0.45
1:B:3:ILE:HD13	1:B:13:LEU:HB2	1.99	0.45
1:B:80:LYS:HD2	1:F:71:GLU:HB3	1.98	0.45
1:C:160:LYS:N	1:C:172:ASP:OD2	2.50	0.45
1:E:261:ALA:HB3	1:E:273:ILE:HG23	1.99	0.45
2:G:44:ARG:HG3	2:G:52:ARG:NH2	2.32	0.45
1:A:153:PHE:HB2	1:A:178:ILE:HD13	1.99	0.45
1:B:58:TYR:OH	1:B:97:ASP:HB3	2.17	0.45
1:A:9:ASN:OD1	1:E:338:TYR:OH	2.29	0.44
1:D:234:THR:OG1	1:D:254:THR:HG22	2.17	0.44
1:E:127:ASP:O	1:E:130:VAL:HG22	2.17	0.44
2:G:167:GLY:O	2:G:171:VAL:HG23	2.16	0.44
2:G:37:ARG:HB3	2:G:37:ARG:HE	1.58	0.44
1:A:18:VAL:HG22	1:A:337:VAL:HG22	1.98	0.44
1:C:96:PHE:CE1	1:C:137:ALA:HB1	2.52	0.44
1:D:12:ASP:O	1:D:45:PHE:HA	2.17	0.44
1:F:109:LEU:HA	1:F:230:ASN:ND2	2.32	0.44
1:C:115:LEU:HG	1:C:119:GLY:HA2	1.99	0.44
1:D:262:GLN:NE2	1:D:272:SER:HB2	2.33	0.44
1:A:132:ARG:HH21	1:E:71:GLU:CD	2.21	0.44
1:B:306:ASN:OD1	1:D:9:ASN:ND2	2.51	0.44
1:E:102:TYR:CE1	1:E:132:ARG:HG3	2.53	0.44
1:E:303:PHE:HB2	1:E:307:MET:HB3	1.99	0.44
1:E:265:PHE:HE2	1:E:271:PRO:HG2	1.83	0.44
2:G:154:TYR:HD2	2:G:155:PRO:HG2	1.83	0.44
2:H:188:ARG:HD3	2:H:188:ARG:HA	1.84	0.44
1:B:295:PHE:HD2	1:B:317:GLN:HE21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLU:HG2	1:D:255:GLN:HG2	1.99	0.44
1:E:267:PHE:CD1	2:H:109:LEU:HD11	2.53	0.44
1:A:252:ASN:ND2	1:A:284:GLU:OE1	2.48	0.43
1:A:263:TYR:O	1:A:271:PRO:HD2	2.18	0.43
1:B:63:TYR:OH	1:F:76:GLN:NE2	2.33	0.43
1:C:95:SER:O	1:C:139:TYR:HA	2.18	0.43
1:F:20:LEU:HD23	1:F:38:MET:HB2	2.00	0.43
1:B:52:ASN:ND2	2:G:104:MET:O	2.46	0.43
2:H:26:PHE:CD1	3:H:301:C8E:H72	2.52	0.43
1:E:265:PHE:CZ	2:H:81:MET:HG3	2.53	0.43
1:A:242:ASN:HD22	1:A:324:LEU:HD23	1.84	0.43
1:B:24:SER:HB2	1:B:35:ASN:HB2	2.00	0.43
1:A:307:MET:HG2	1:C:88:LEU:HD21	2.00	0.43
1:A:80:LYS:HD2	1:E:71:GLU:HB3	2.00	0.43
2:H:37:ARG:HG2	2:H:177:ARG:HH12	1.82	0.43
1:A:263:TYR:CZ	3:A:401:C8E:H61	2.54	0.43
1:E:18:VAL:HG12	1:E:20:LEU:HB2	2.00	0.43
2:H:37:ARG:HE	2:H:37:ARG:HB3	1.63	0.43
1:A:263:TYR:CD2	3:A:401:C8E:H82	2.54	0.43
2:G:41:VAL:HG22	2:G:181:LEU:HD13	1.99	0.43
2:H:172:GLU:O	2:H:176:THR:OG1	2.27	0.43
1:C:286:ILE:HG23	1:C:323:LYS:HD2	2.01	0.43
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.88	0.43
1:D:279:LYS:NZ	1:D:288:ASP:HB3	2.34	0.43
1:F:89:LYS:HE3	1:F:95:SER:HB3	2.00	0.43
1:C:223:ASN:O	1:C:225:ILE:HG13	2.18	0.43
2:G:170:VAL:O	2:G:174:ILE:HG13	2.18	0.43
1:B:116:PRO:HD2	1:B:312:ASP:OD1	2.19	0.43
1:C:22:TYR:HD2	1:C:33:GLY:O	2.02	0.43
1:D:314:ILE:O	1:D:330:ASP:HB2	2.18	0.43
1:A:115:LEU:HD13	1:A:296:GLU:HG3	2.01	0.43
1:A:309:THR:HG22	1:A:336:ILE:HA	2.01	0.43
1:D:164:ASP:N	1:D:164:ASP:OD2	2.52	0.43
1:A:95:SER:OG	1:A:140:ARG:HB2	2.19	0.42
1:B:46:LYS:HG2	1:B:60:GLN:CD	2.40	0.42
1:D:330:ASP:OD1	1:D:330:ASP:N	2.41	0.42
1:E:111:TYR:CZ	1:E:219:LYS:HD3	2.53	0.42
1:E:223:ASN:HB2	1:E:225:ILE:HD12	2.00	0.42
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.55	0.42
1:E:242:ASN:HB2	1:E:324:LEU:HD23	1.98	0.42
2:G:163:TRP:O	2:G:166:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:MET:HG3	2:H:80:GLY:O	2.20	0.42
1:A:289:VAL:HG11	1:A:324:LEU:HG	2.01	0.42
1:B:205:LEU:HB2	1:B:249:GLY:HA3	2.01	0.42
1:B:20:LEU:HD23	1:B:38:MET:O	2.18	0.42
1:C:153:PHE:HA	1:C:177:SER:O	2.19	0.42
1:D:58:TYR:OH	1:D:97:ASP:HB3	2.20	0.42
1:E:138:THR:OG1	1:E:156:GLN:NE2	2.48	0.42
1:E:334:VAL:HG11	2:H:92:LEU:HD11	2.00	0.42
2:G:117:PHE:HD2	2:G:150:ALA:HB3	1.84	0.42
1:C:54:ASP:HB3	1:C:90:TYR:CE1	2.55	0.42
1:B:189:GLY:HA2	1:B:216:THR:HA	2.02	0.42
2:G:117:PHE:HD1	2:G:120:THR:HB	1.84	0.42
1:B:191:TYR:CD1	1:B:214:TRP:HB3	2.53	0.42
2:H:28:TYR:HH	2:H:187:LEU:HB3	1.84	0.42
1:D:14:TYR:CE1	1:D:46:LYS:HG3	2.55	0.42
1:D:277:LYS:HA	1:D:292:VAL:O	2.20	0.42
1:D:98:TYR:CE1	3:D:402:C8E:H41	2.55	0.42
1:E:68:ASN:OD1	1:E:69:ASN:ND2	2.42	0.42
1:B:38:MET:HA	1:B:68:ASN:ND2	2.35	0.41
1:D:109:LEU:HA	1:D:109:LEU:HD23	1.82	0.41
1:E:273:ILE:HD12	1:E:296:GLU:O	2.20	0.41
1:F:61:TRP:NE1	1:F:81:THR:HG23	2.35	0.41
2:H:69:VAL:CG1	2:H:154:TYR:CE1	3.03	0.41
1:A:286:ILE:HG23	1:A:323:LYS:HE3	2.01	0.41
1:F:113:ASP:OD1	1:F:120:GLY:HA3	2.20	0.41
2:G:132:VAL:HG12	2:G:133:MET:N	2.35	0.41
2:H:132:VAL:HG12	2:H:133:MET:N	2.35	0.41
1:A:257:VAL:C	1:A:258:LEU:HD12	2.41	0.41
1:A:273:ILE:HA	1:A:296:GLU:O	2.21	0.41
1:A:40:TYR:HA	1:A:67:GLY:H	1.85	0.41
1:C:276:THR:HB	1:C:294:TYR:CZ	2.56	0.41
1:D:208:GLY:HA3	1:D:236:ASN:ND2	2.35	0.41
1:E:25:LYS:HD2	1:E:25:LYS:C	2.41	0.41
1:F:122:THR:HA	1:F:124:TYR:CE1	2.55	0.41
1:F:204:PRO:HD2	1:F:248:SER:O	2.21	0.41
2:H:147:GLY:C	2:H:149:PHE:H	2.24	0.41
1:A:178:ILE:O	1:A:188:VAL:HG23	2.19	0.41
1:C:5:ASN:O	1:C:6:LYS:HD3	2.20	0.41
1:E:173:GLY:HA3	1:E:194:ALA:HB2	2.03	0.41
2:G:63:GLU:O	2:G:67:SER:OG	2.31	0.41
2:H:149:PHE:O	2:H:149:PHE:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:ARG:HG2	2:H:177:ARG:NH1	2.36	0.41
1:A:238:THR:HB	1:A:254:THR:HG21	2.03	0.41
1:B:22:TYR:CD2	1:B:38:MET:HG3	2.56	0.41
1:B:69:ASN:HB3	1:B:75:ALA:HA	2.03	0.41
1:E:5:ASN:O	1:E:6:LYS:HD3	2.20	0.41
2:G:134:LEU:HD23	2:G:140:PHE:HB2	2.02	0.41
2:G:98:LEU:H	2:G:98:LEU:HD12	1.85	0.41
2:H:147:GLY:C	2:H:149:PHE:N	2.74	0.41
2:H:73:LEU:HD23	2:H:73:LEU:HA	1.80	0.41
1:B:6:LYS:HD3	1:B:6:LYS:HA	1.63	0.41
1:F:225:ILE:HG12	1:F:263:TYR:CD1	2.55	0.41
1:B:47:GLY:HA3	1:F:338:TYR:CZ	2.56	0.41
2:H:134:LEU:HB2	2:H:137:TYR:HB3	2.01	0.41
1:A:161:ASN:HB2	1:A:170:ASN:OD1	2.21	0.41
1:A:111:TYR:CE1	1:A:219:LYS:HD3	2.55	0.41
1:B:285:GLY:C	1:B:286:ILE:HD12	2.41	0.41
1:C:174:VAL:HG12	1:C:175:GLY:N	2.35	0.41
1:D:158:LEU:O	1:D:172:ASP:HA	2.21	0.41
1:E:218:LEU:O	1:E:228:ALA:HA	2.20	0.41
1:A:216:THR:O	1:A:230:ASN:HA	2.20	0.41
1:B:27:ASN:OD1	1:B:29:GLU:HB2	2.20	0.41
1:B:12:ASP:O	1:B:45:PHE:HA	2.21	0.41
1:F:301:TYR:C	1:F:301:TYR:CD1	2.94	0.41
2:H:134:LEU:HD23	2:H:140:PHE:HB2	2.02	0.41
1:F:233:GLU:HG2	1:F:255:GLN:HG2	2.02	0.41
2:G:74:LYS:NZ	2:G:120:THR:OG1	2.54	0.41
2:G:201:TYR:CD1	2:G:201:TYR:C	2.93	0.41
1:A:82:ARG:O	1:A:83:LEU:HD23	2.21	0.41
1:C:305:LYS:HG3	1:C:306:ASN:ND2	2.36	0.41
1:C:51:ILE:HG21	1:C:55:LEU:HD23	2.03	0.41
1:F:107:ASP:OD2	1:F:140:ARG:NH1	2.44	0.41
1:F:1:ALA:N	1:F:13:LEU:O	2.44	0.41
2:G:86:ARG:CZ	2:G:111:ARG:HG2	2.51	0.41
1:A:231:TYR:OH	1:A:233:GLU:OE2	2.35	0.40
1:D:23:PHE:HB2	1:D:332:VAL:HG13	2.02	0.40
1:D:295:PHE:HZ	3:D:401:C8E:H71	1.86	0.40
2:G:154:TYR:HB2	2:G:155:PRO:CD	2.44	0.40
1:A:20:LEU:HD23	1:A:38:MET:HB2	2.02	0.40
1:B:84:ALA:O	1:B:99:GLY:HA3	2.21	0.40
1:C:18:VAL:HG13	1:C:337:VAL:HG22	2.03	0.40
1:F:219:LYS:HA	1:F:227:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:TYR:HD1	1:C:174:VAL:HG22	1.87	0.40
1:C:300:THR:HB	1:C:302:TYR:CE2	2.56	0.40
1:E:69:ASN:OD1	1:E:77:THR:HB	2.21	0.40
1:F:217:GLY:HA2	1:F:230:ASN:OD1	2.22	0.40
1:F:301:TYR:HE1	1:F:303:PHE:HA	1.86	0.40
2:G:70:ASN:O	2:G:74:LYS:HG3	2.22	0.40
2:H:52:ARG:O	2:H:55:ILE:HG13	2.22	0.40
1:A:122:THR:HA	1:A:124:TYR:HE1	1.87	0.40
1:B:20:LEU:HD13	1:B:310:TYR:OH	2.21	0.40
1:B:84:ALA:O	1:B:100:ARG:N	2.48	0.40
1:C:96:PHE:HE1	1:C:137:ALA:HB1	1.86	0.40
1:E:27:ASN:OD1	1:E:29:GLU:N	2.46	0.40
1:F:45:PHE:CE2	1:F:61:TRP:HB3	2.56	0.40
2:G:123:HIS:HD1	2:G:124:TYR:HD1	1.69	0.40
1:A:28:GLY:O	1:A:31:SER:HB3	2.21	0.40
1:C:102:TYR:CZ	1:C:132:ARG:HG3	2.56	0.40
1:C:303:PHE:HB2	1:C:307:MET:HB3	2.03	0.40
1:C:82:ARG:O	1:C:83:LEU:HD23	2.22	0.40
1:E:109:LEU:HD23	1:E:109:LEU:HA	1.92	0.40
1:E:220:TYR:O	1:E:226:TYR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	318 (94%)	20 (6%)	0	100	100
1	B	338/340 (99%)	317 (94%)	21 (6%)	0	100	100
1	C	338/340 (99%)	318 (94%)	19 (6%)	1 (0%)	41	74
1	D	338/340 (99%)	317 (94%)	20 (6%)	1 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	338/340 (99%)	317 (94%)	19 (6%)	2 (1%)	25 64
1	F	338/340 (99%)	318 (94%)	19 (6%)	1 (0%)	41 74
2	G	198/235 (84%)	170 (86%)	21 (11%)	7 (4%)	3 24
2	H	197/235 (84%)	167 (85%)	26 (13%)	4 (2%)	7 38
All	All	2423/2510 (96%)	2242 (92%)	165 (7%)	16 (1%)	22 61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	GLY
2	G	36	LEU
2	G	155	PRO
2	G	161	THR
1	D	120	GLY
2	H	13	SER
1	E	120	GLY
2	G	135	PRO
2	H	135	PRO
2	H	146	GLY
1	E	91	ALA
1	F	120	GLY
2	G	12	ARG
2	G	146	GLY
2	H	68	MET
2	G	15	PRO

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	263/263 (100%)	260 (99%)	3 (1%)	73 88
1	B	263/263 (100%)	259 (98%)	4 (2%)	65 85
1	C	263/263 (100%)	258 (98%)	5 (2%)	57 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	263/263 (100%)	259 (98%)	4 (2%)	65 85
1	E	263/263 (100%)	261 (99%)	2 (1%)	81 93
1	F	263/263 (100%)	258 (98%)	5 (2%)	57 81
2	G	167/195 (86%)	160 (96%)	7 (4%)	30 65
2	H	167/195 (86%)	156 (93%)	11 (7%)	16 51
All	All	1912/1968 (97%)	1871 (98%)	41 (2%)	53 79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TYR
1	A	100	ARG
1	A	313	TYR
1	B	42	ARG
1	B	100	ARG
1	B	312	ASP
1	B	313	TYR
1	C	20	LEU
1	C	60	GLN
1	C	100	ARG
1	C	312	ASP
1	C	320	SER
1	D	20	LEU
1	D	179	SER
1	D	290	ASP
1	D	312	ASP
1	E	25	LYS
1	E	107	ASP
1	F	50	GLN
1	F	179	SER
1	F	266	ASP
1	F	272	SER
1	F	312	ASP
2	G	46	TYR
2	G	88	PHE
2	G	111	ARG
2	G	117	PHE
2	G	177	ARG
2	G	190	SER
2	G	196	MET

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Mol	Chain	Res	Type
2	H	23	MET
2	H	45	ASP
2	H	88	PHE
2	H	111	ARG
2	H	149	PHE
2	H	154	TYR
2	H	177	ARG
2	H	188	ARG
2	H	192	ASP
2	H	207	PHE
2	H	210	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN
1	D	9	ASN
1	D	306	ASN
1	E	69	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

9 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	$\#\|Z\| > 2$
3	C8E	A	402	-	11,11,20	0.38	0	10,10,19	0.49	0
3	C8E	D	401	-	10,10,20	0.33	0	9,9,19	0.58	0
3	C8E	B	402	-	8,8,20	0.24	0	7,7,19	0.44	0
3	C8E	B	401	-	8,8,20	0.50	0	7,7,19	0.21	0
3	C8E	D	402	-	8,8,20	0.23	0	7,7,19	0.35	0
3	C8E	H	302	-	12,12,20	0.38	0	11,11,19	0.32	0
3	C8E	H	301	-	10,10,20	0.37	0	9,9,19	0.56	0
3	C8E	A	401	-	8,8,20	0.39	0	7,7,19	0.31	0
3	C8E	F	401	-	8,8,20	0.20	0	7,7,19	0.64	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	A	402	-	-	3/9/9/18	-
3	C8E	D	401	-	-	3/8/8/18	-
3	C8E	B	402	-	-	4/6/6/18	-
3	C8E	B	401	-	-	4/6/6/18	-
3	C8E	D	402	-	-	4/6/6/18	-
3	C8E	H	302	-	-	5/10/10/18	-
3	C8E	H	301	-	-	4/8/8/18	-
3	C8E	A	401	-	-	4/6/6/18	-
3	C8E	F	401	-	-	4/6/6/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	C8E	C4-C5-C6-C7
3	H	302	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
3	H	301	C8E	C3-C4-C5-C6
3	H	302	C8E	C6-C7-C8-O9
3	H	301	C8E	C4-C5-C6-C7
3	A	402	C8E	C3-C4-C5-C6
3	F	401	C8E	C3-C4-C5-C6
3	H	301	C8E	C6-C7-C8-O9
3	D	402	C8E	C5-C6-C7-C8
3	B	402	C8E	C4-C5-C6-C7
3	H	301	C8E	C2-C3-C4-C5
3	B	402	C8E	C2-C3-C4-C5
3	D	401	C8E	C5-C6-C7-C8
3	F	401	C8E	C5-C6-C7-C8
3	B	402	C8E	C3-C4-C5-C6
3	A	401	C8E	C6-C7-C8-O9
3	B	401	C8E	C13-C14-O15-C16
3	H	302	C8E	C3-C4-C5-C6
3	A	401	C8E	C3-C4-C5-C6
3	B	402	C8E	C7-C8-O9-C10
3	F	401	C8E	C1-C2-C3-C4
3	D	402	C8E	C2-C3-C4-C5
3	D	401	C8E	C7-C8-O9-C10
3	B	401	C8E	O18-C19-C20-O21
3	B	401	C8E	O15-C16-C17-O18
3	D	401	C8E	C4-C5-C6-C7
3	H	302	C8E	C2-C3-C4-C5
3	A	401	C8E	C7-C8-O9-C10
3	B	401	C8E	C20-C19-O18-C17
3	A	401	C8E	C11-C10-O9-C8
3	D	402	C8E	C7-C8-O9-C10
3	F	401	C8E	C4-C5-C6-C7
3	A	402	C8E	C7-C8-O9-C10
3	A	402	C8E	C4-C5-C6-C7
3	H	302	C8E	C10-C11-O12-C13

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	C8E	1	0
3	D	401	C8E	1	0
3	D	402	C8E	3	0
3	H	302	C8E	2	0

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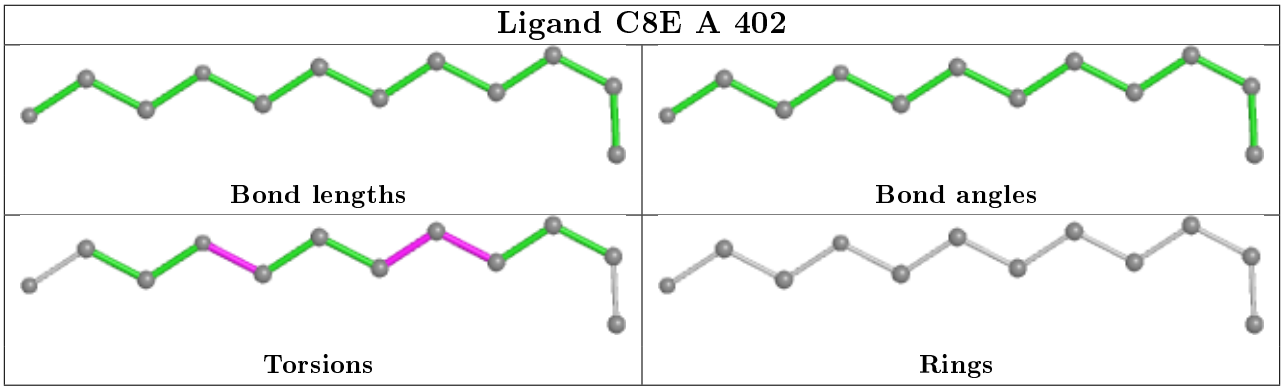
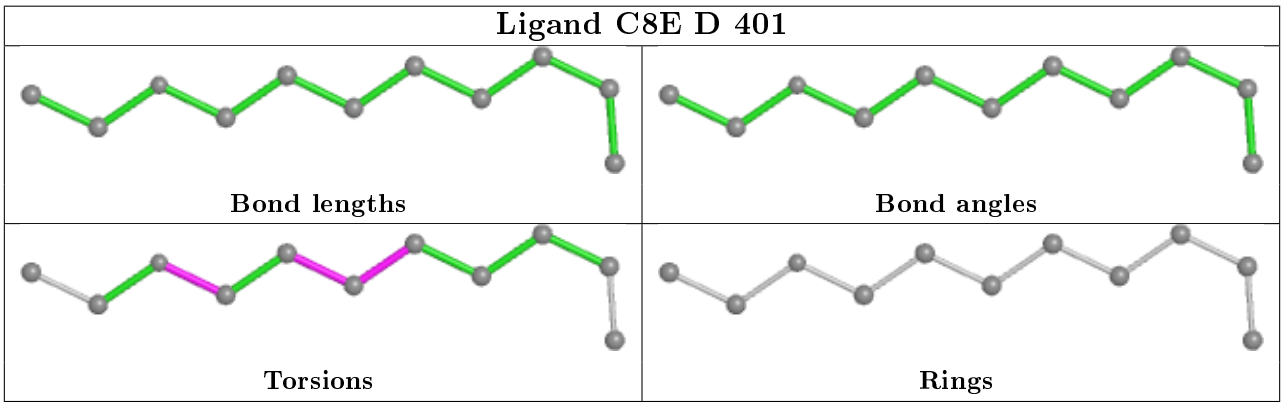
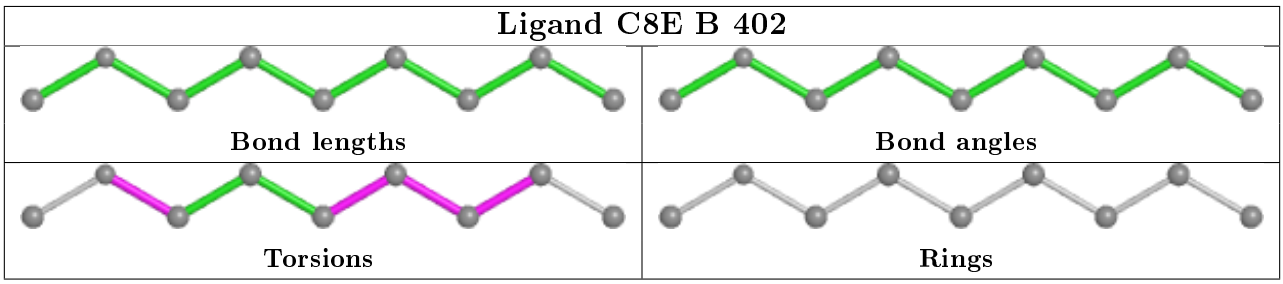
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	C8E	1	0
3	A	401	C8E	3	0

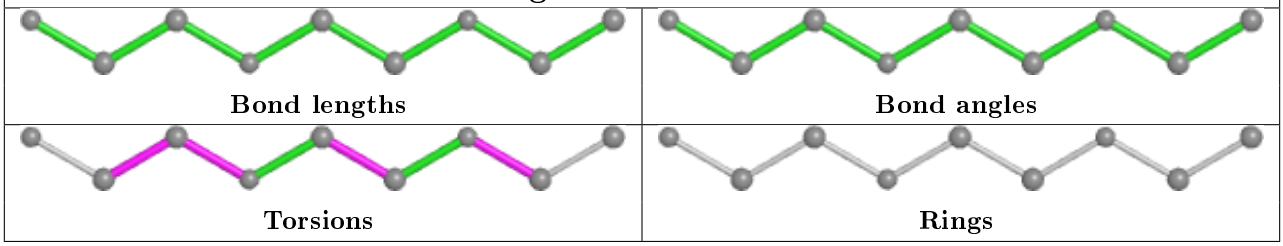
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



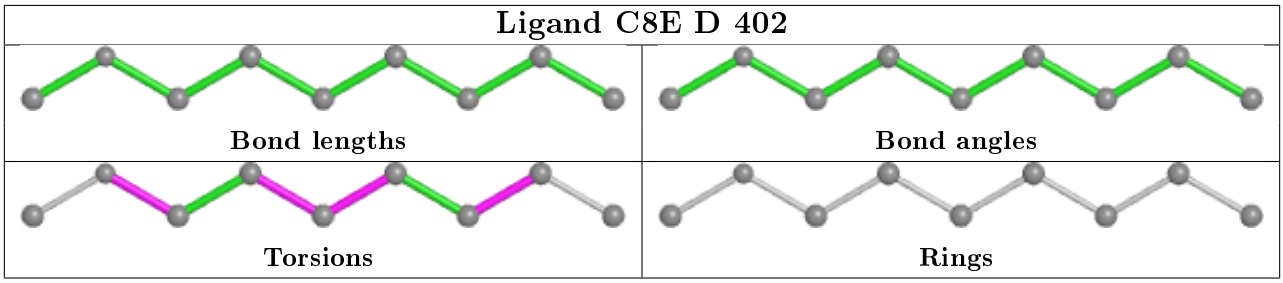




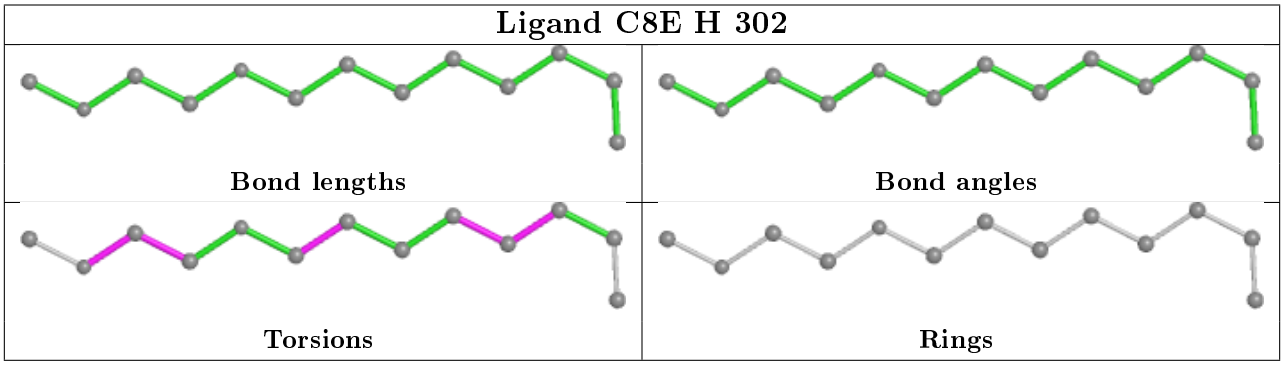
Ligand C8E B 401



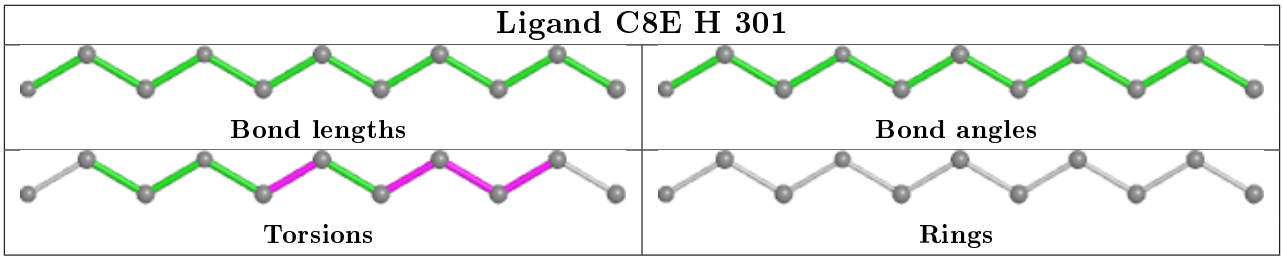
Ligand C8E D 402



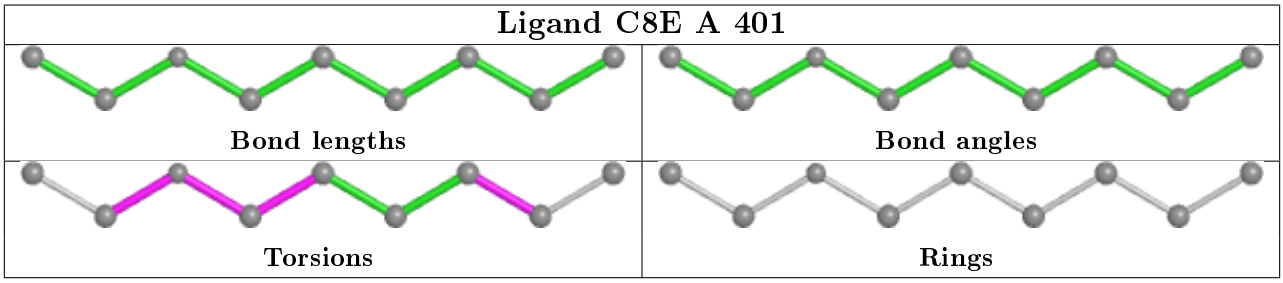
Ligand C8E H 302

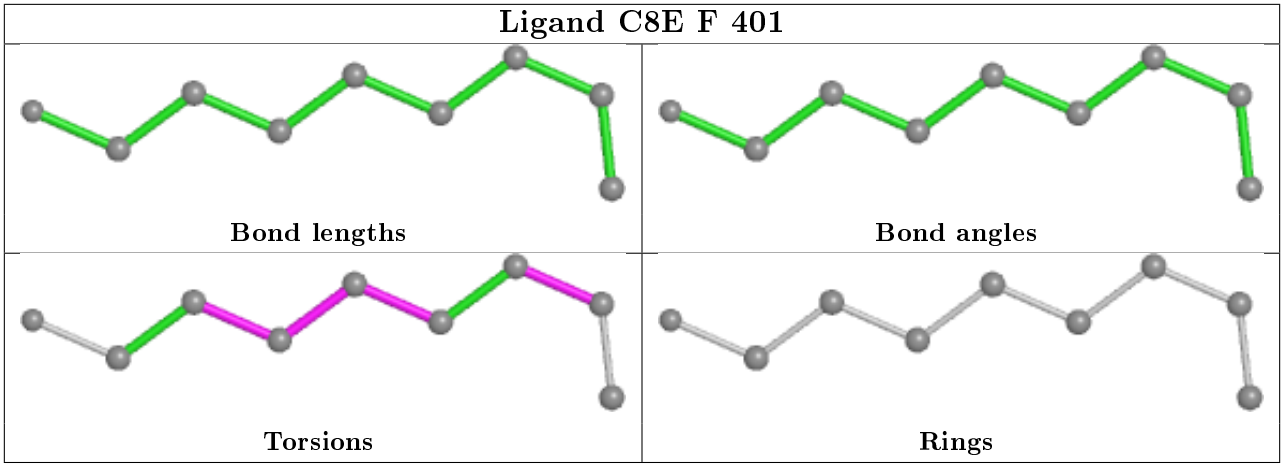


Ligand C8E H 301



Ligand C8E A 401





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, 95^{th} 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	340/340 (100%)	-0.12	0 100 100	26, 38, 60, 84	0
1	B	340/340 (100%)	-0.03	1 (0%) 94 92	26, 37, 60, 77	0
1	C	340/340 (100%)	0.08	1 (0%) 94 92	25, 41, 64, 100	0
1	D	340/340 (100%)	-0.02	0 100 100	24, 38, 64, 92	0
1	E	340/340 (100%)	0.17	2 (0%) 89 83	25, 52, 77, 101	0
1	F	340/340 (100%)	0.17	2 (0%) 89 83	25, 48, 70, 84	0
2	G	200/235 (85%)	0.36	9 (4%) 33 21	36, 58, 88, 107	0
2	H	199/235 (84%)	0.23	2 (1%) 82 72	29, 53, 83, 97	0
All	All	2439/2510 (97%)	0.08	17 (0%) 87 81	24, 45, 71, 107	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	155	PRO	5.5
2	G	159	TYR	3.5
2	H	155	PRO	3.3
2	G	28	TYR	3.2
2	G	156	MET	2.8
2	G	181	LEU	2.7
2	G	163	TRP	2.5
2	G	157	LEU	2.5
2	G	188	ARG	2.3
2	H	163	TRP	2.2
1	E	84	ALA	2.1
1	B	178	ILE	2.0
1	F	308	SER	2.0
1	F	34	GLY	2.0
1	C	339	GLN	2.0
2	G	210	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	203	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

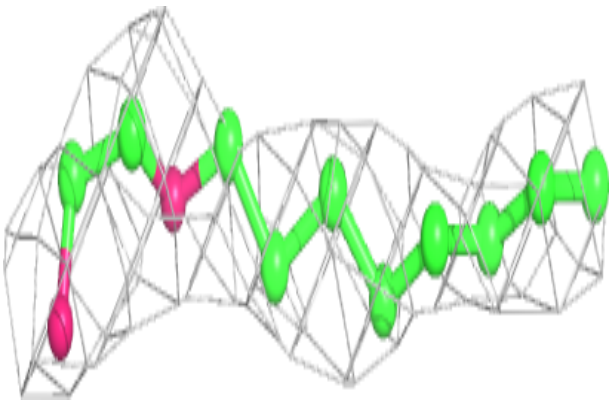
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

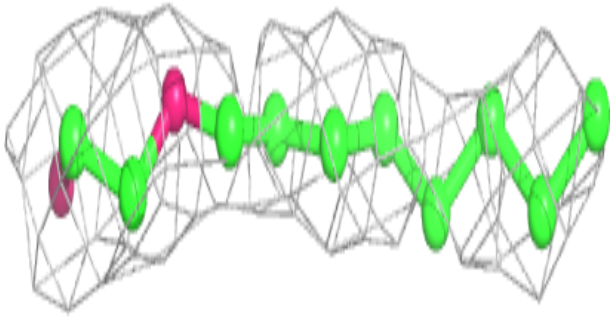
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C8E	A	402	12/21	0.90	0.42	35,44,50,51	0
3	C8E	H	302	13/21	0.91	0.25	39,43,49,51	0
3	C8E	H	301	11/21	0.91	0.25	23,30,37,39	0
3	C8E	B	402	9/21	0.93	0.23	17,21,24,26	0
3	C8E	D	401	11/21	0.94	0.21	6,14,33,33	0
3	C8E	B	401	9/21	0.95	0.18	13,31,37,38	0
3	C8E	A	401	9/21	0.95	0.18	7,18,28,28	0
3	C8E	F	401	9/21	0.95	0.36	19,21,33,35	0
3	C8E	D	402	9/21	0.97	0.28	13,21,28,29	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:

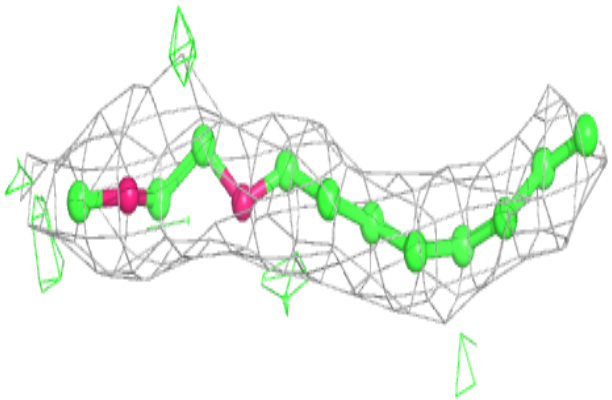
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

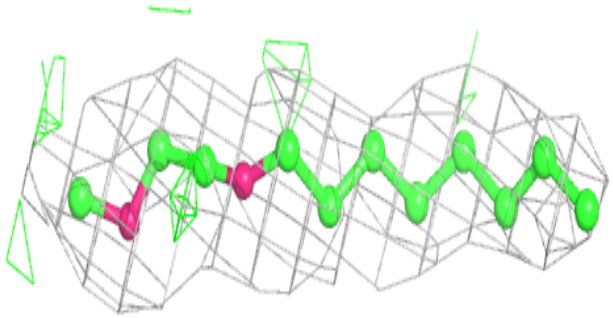


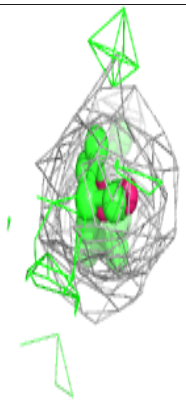


Electron density around C8E H 302:

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

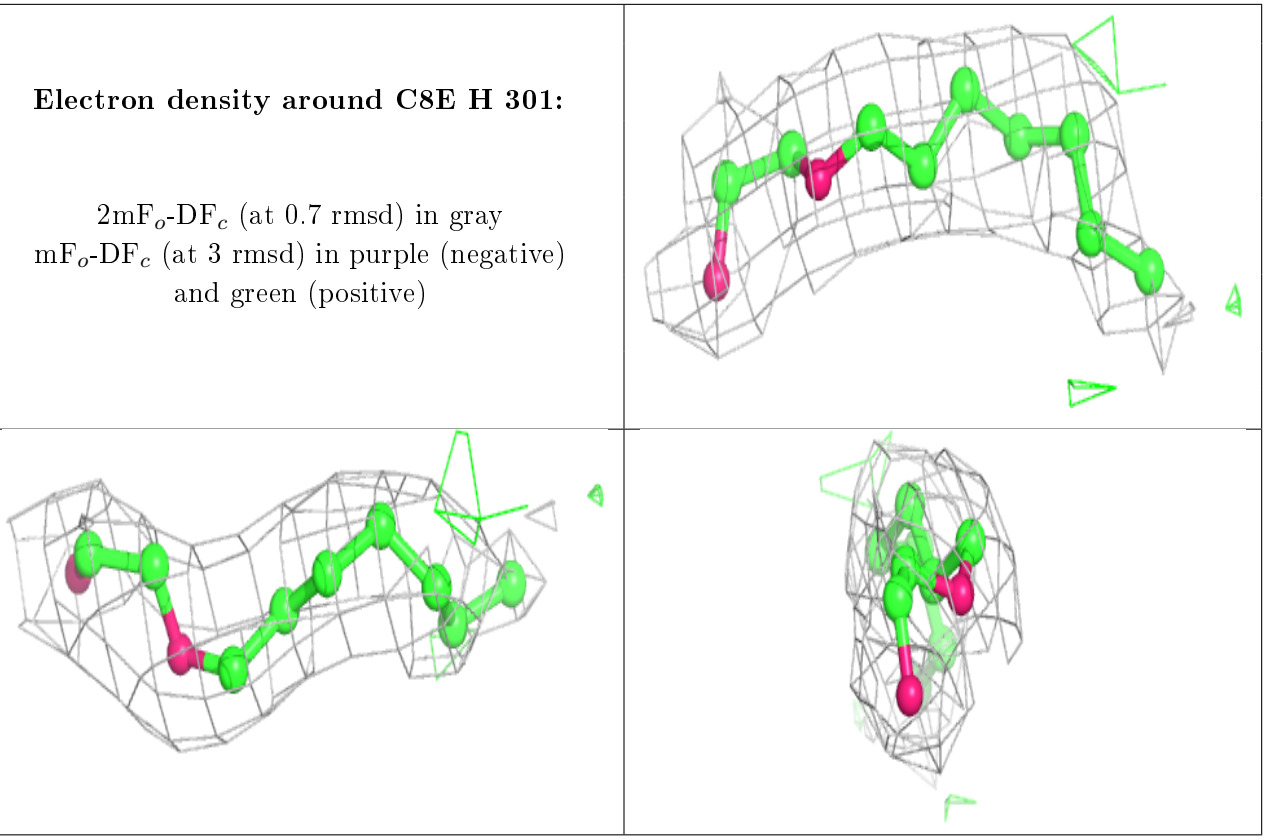






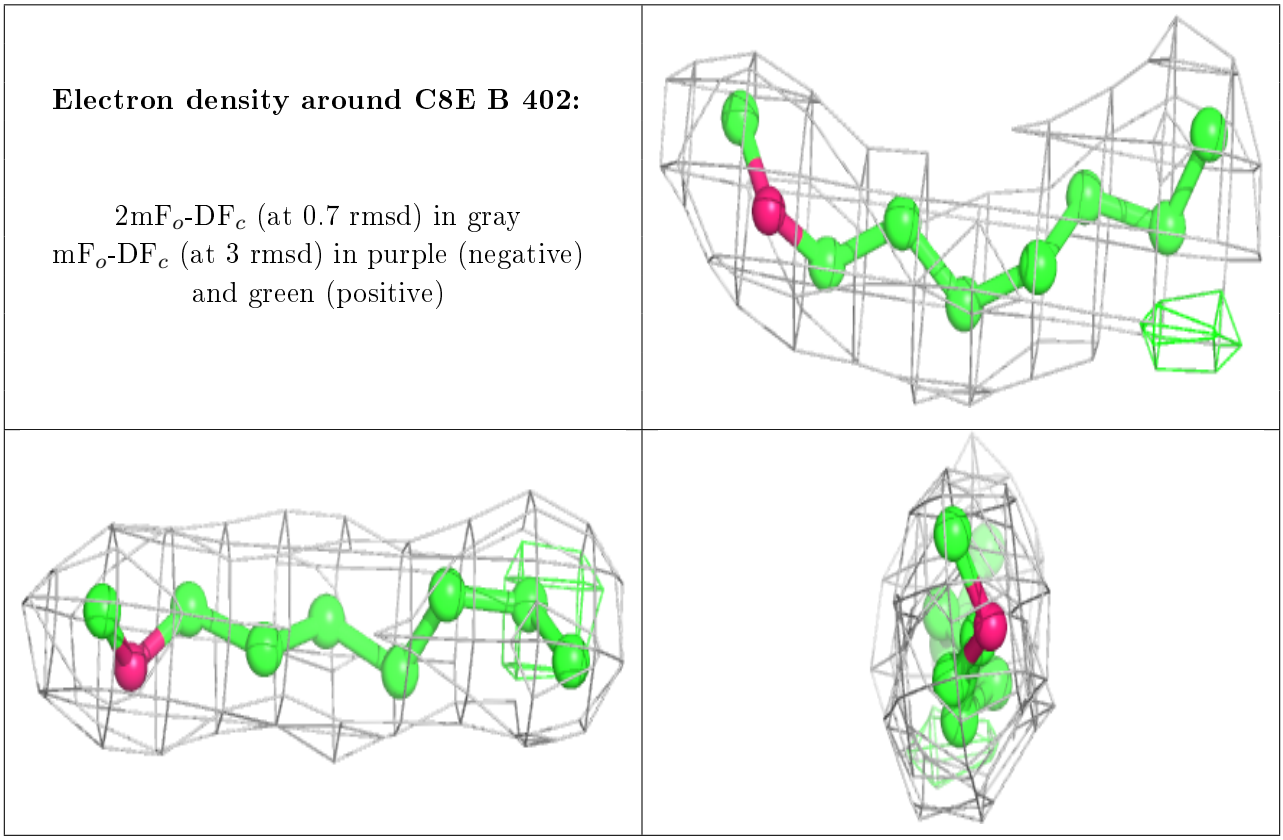
Electron density around C8E H 301:

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



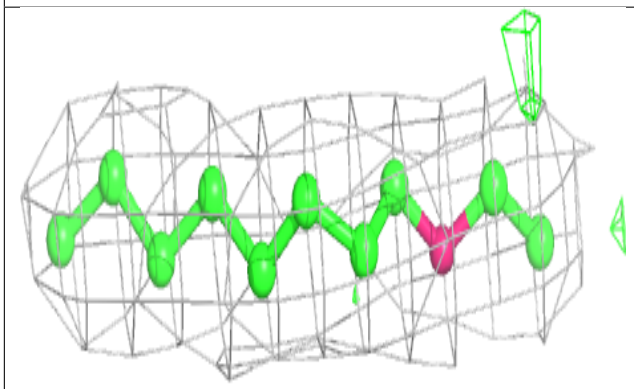
Electron density around C8E B 402:

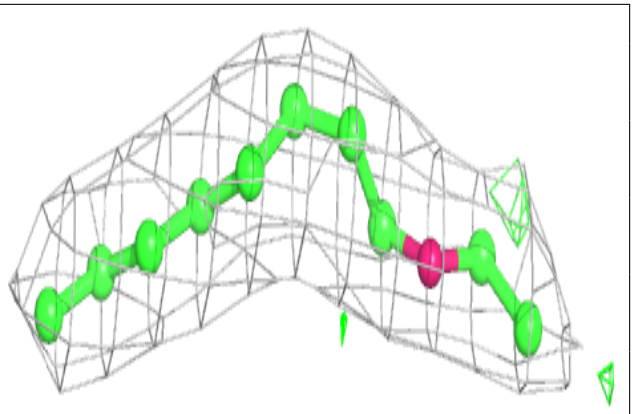
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

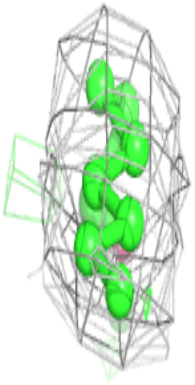


Electron density around C8E D 401:

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

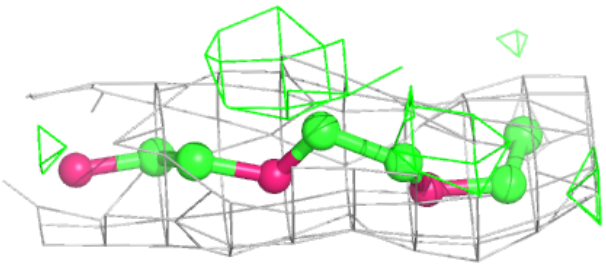


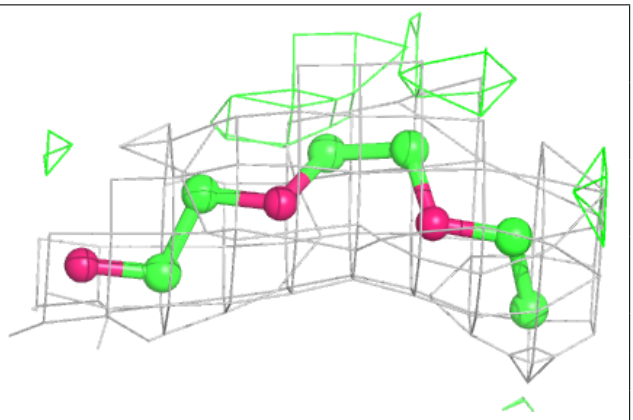


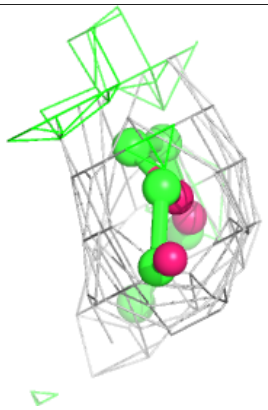


Electron density around C8E B 401:

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

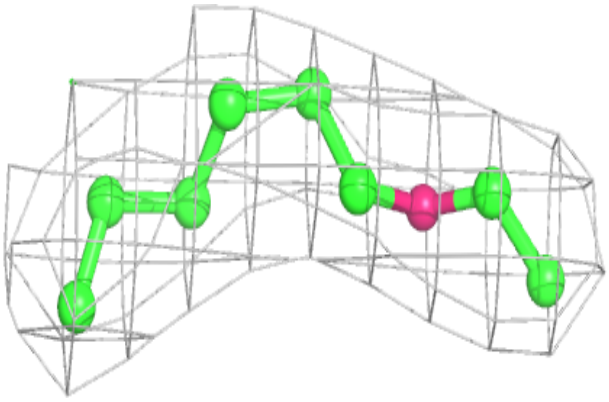


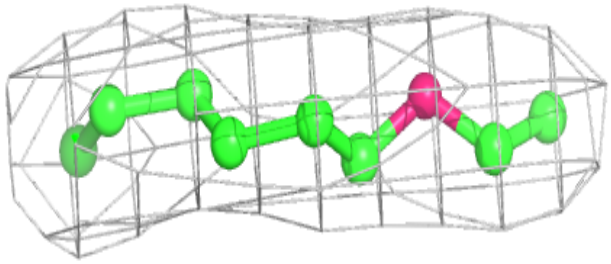


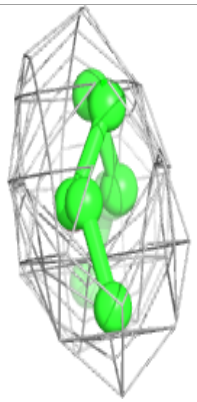


Electron density around C8E A 401:

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

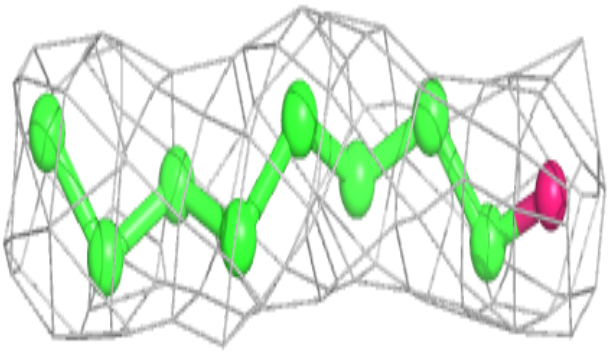


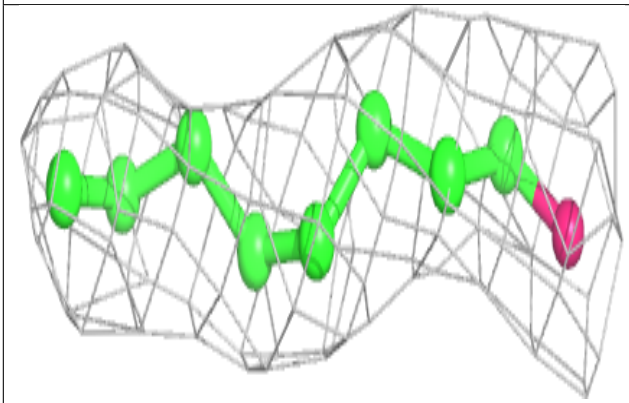


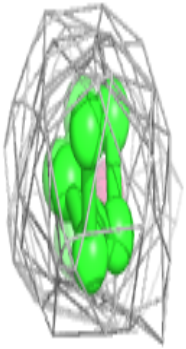


Electron density around C8E F 401:

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

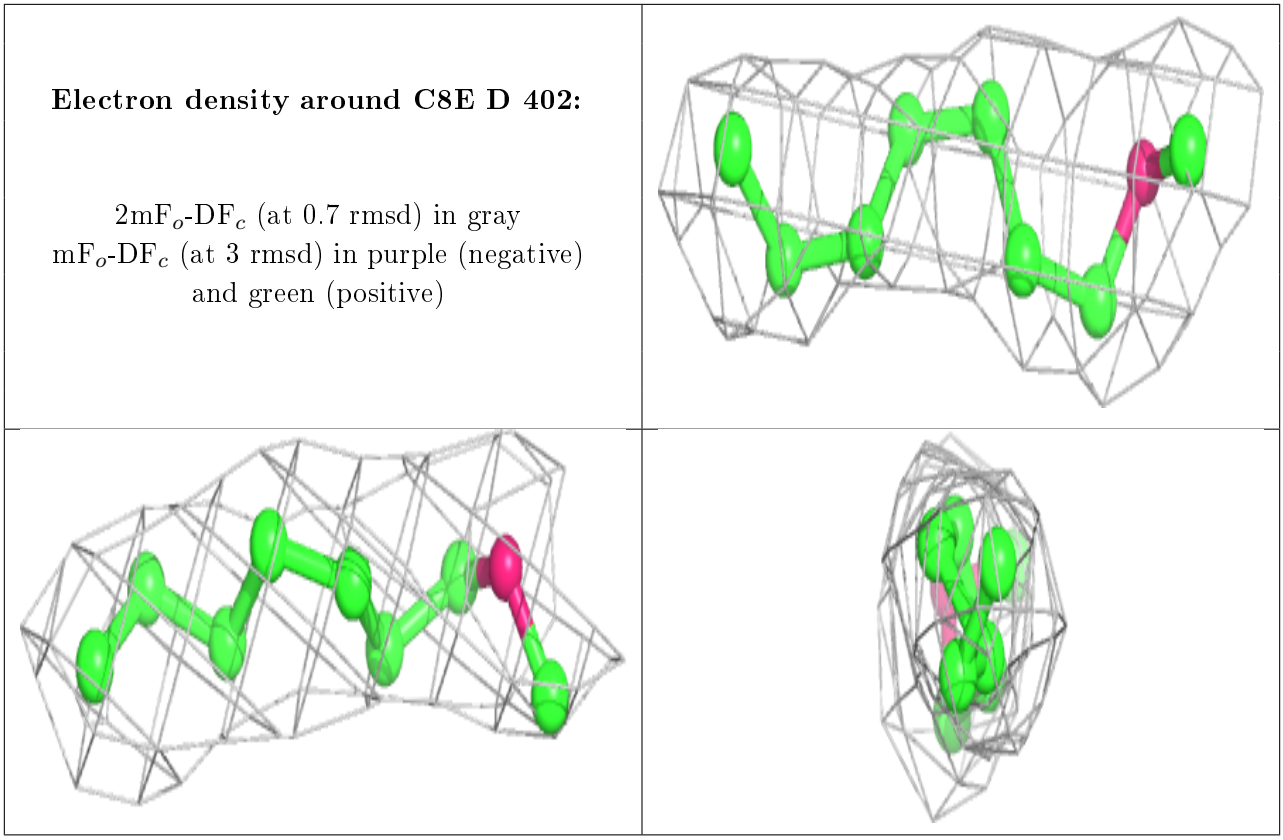






Electron density around C8E D 402:

$2mF_o$-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.