Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2023 – 03:00 AM EDT

PDB ID	:	3VG9
Title	:	Crystal structure of human adenosine A2A receptor with an allosteric inverse-agonist antibody at 2.7 A resolution
Authors	:	Hino, T.; Arakawa, T.; Iwanari, H.; Yurugi-Kobayashi, T.; Ikeda-Suno, C.; Nakada-Nakura, Y.; Kusano-Arai, O.; Weyand, S.; Shimamura, T.; Nomura, N.; Cameron, A.D.; Kobayashi, T.; Hamakubo, T.; Iwata, S.; Murata, T.
Deposited on	:	2011-08-04
Resolution	:	2.70 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 (1)) were used in the production of this report:

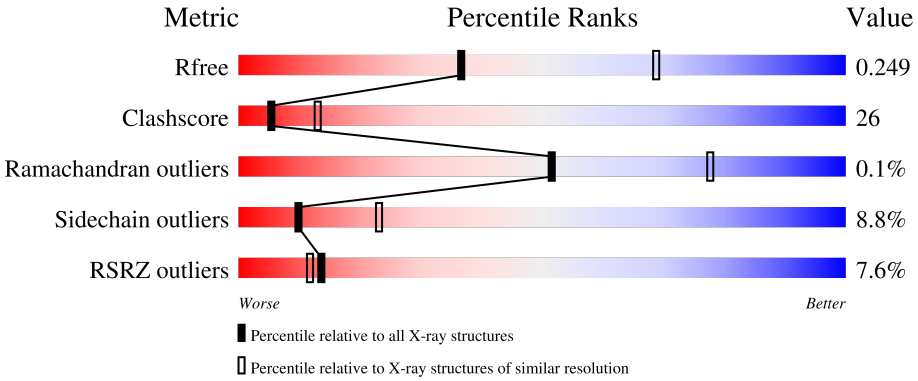
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	326	15% 41% 41% 9% 9%
2	B	214	2% 71% 29%
3	C	226	% 78% 19%

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
5	STE	A	402	-	-	-	X
5	STE	A	405	-	-	-	X
5	STE	A	407	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5901 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 Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2318	1529	388	381	20	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLN	ASN	engineered mutation	UNP P29274
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

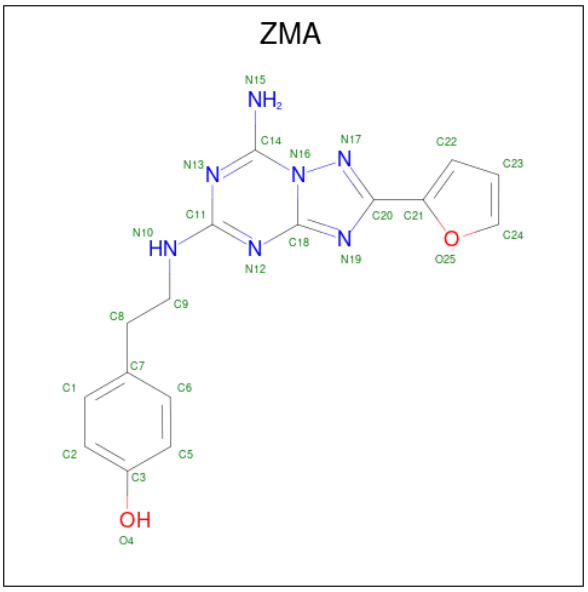
- Molecule 2 is a protein called antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1639	1026	275	332	6	0	0	0

- Molecule 3 is a protein called antibody fab fragment heavy chain.

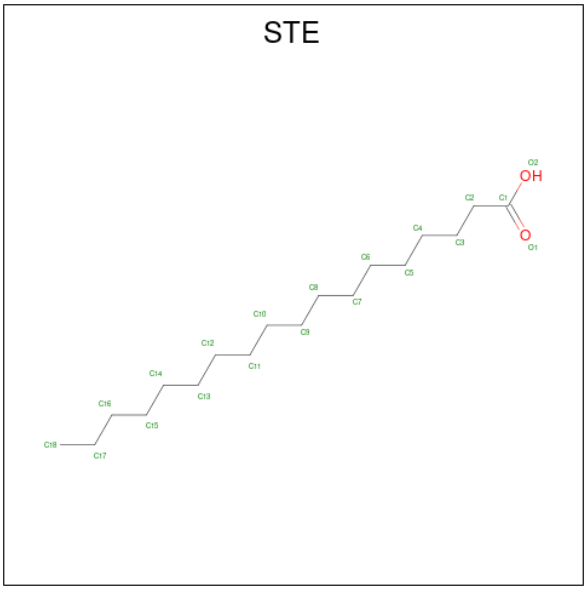
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	224	1694	1067	279	342	6	0	0	0

- Molecule 4 is 4-{2-[(7-amino-2-furan-2-yl[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: $C_{16}H_{15}N_7O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 5 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			20	18	2			
5	A	1	Total	C	O		0	0
			20	18	2			
5	A	1	Total	C	O		0	0
			20	18	2			

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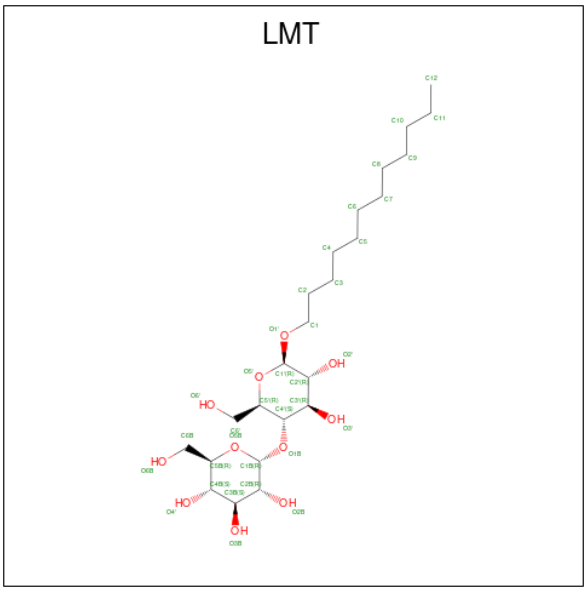
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 20 18 2	0	0

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 35 24 11	0	0

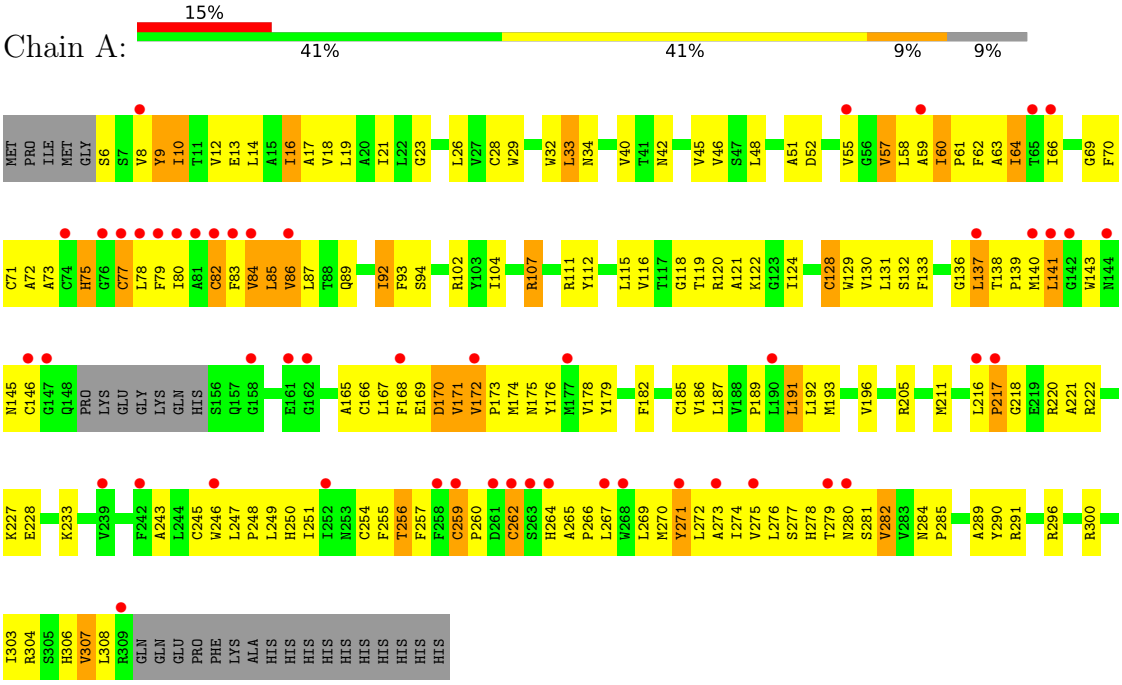
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	B	24	Total O 24 24	0	0
7	C	39	Total O 39 39	0	0

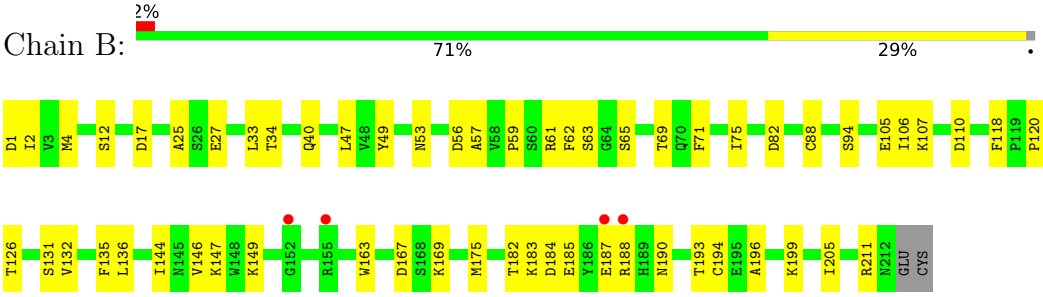
3 Residue-property plots (i)

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.

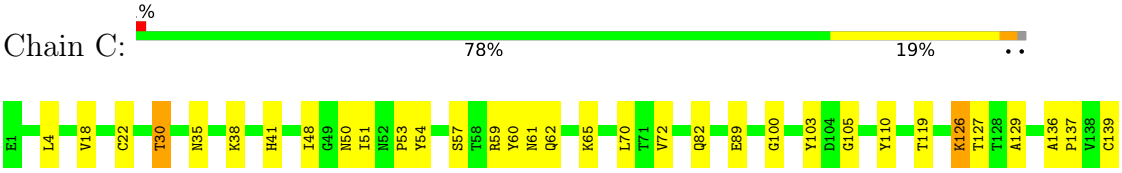
• Molecule 1: Adenosine receptor A2a

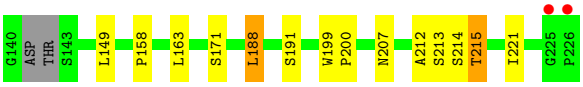


• Molecule 2: antibody fab fragment light chain



• Molecule 3: antibody fab fragment heavy chain




G140
ASP
THR
S143
L149
P158
L163
S171
L188
S191
W199
P200
N207
A212
S213
S214
T215
I221
G225
P226

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.18Å 90.15Å 113.55Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 63.15 – 2.44	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-2.70) 92.3 (63.15-2.44)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.206 , 0.246 0.206 , 0.249	Depositor DCC
R_{free} test set	2114 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 78.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5901	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, STE, ZMA

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	0.30	0/2374	0.49	0/3236
2	B	0.34	0/1678	0.54	0/2280
3	C	0.34	0/1736	0.54	0/2366
All	All	0.33	0/5788	0.52	0/7882

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2318	0	2393	224	0
2	B	1639	0	1562	42	0
3	C	1694	0	1640	35	0
4	A	25	0	15	4	0
5	A	120	0	210	22	0
6	A	35	0	46	1	0
7	A	7	0	0	0	0
7	B	24	0	0	1	0
7	C	39	0	0	1	0
All	All	5901	0	5866	305	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 26.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:CYS:HA	1:A:276:LEU:HD21	1.26	1.17
1:A:259:CYS:SG	1:A:262:CYS:HB2	1.96	1.06
1:A:28:CYS:HB3	5:A:405:STE:H82	1.41	1.02
1:A:69:GLY:HA2	1:A:167:LEU:HD11	1.47	0.97
1:A:143:TRP:CH2	1:A:173:PRO:HG2	2.01	0.95
1:A:62:PHE:CE2	1:A:79:PHE:HE2	1.85	0.94
1:A:259:CYS:SG	1:A:262:CYS:CB	2.55	0.94
1:A:13:GLU:HB3	1:A:60:ILE:HG13	1.48	0.93
1:A:9:TYR:HE2	1:A:64:ILE:HD11	1.34	0.91
1:A:62:PHE:HE2	1:A:79:PHE:HE2	1.16	0.91
1:A:9:TYR:CD2	1:A:10:ILE:HD13	2.06	0.90
1:A:86:VAL:HG21	1:A:133:PHE:CD1	2.08	0.89
1:A:60:ILE:HG22	1:A:61:PRO:HD3	1.51	0.88
1:A:249:LEU:HB2	1:A:273:ALA:HB1	1.56	0.88
1:A:259:CYS:HB3	1:A:262:CYS:HB3	1.54	0.87
1:A:57:VAL:HG13	1:A:58:LEU:HD13	1.57	0.86
1:A:9:TYR:CE2	1:A:64:ILE:HD11	2.11	0.85
1:A:168:PHE:CD2	1:A:172:VAL:HG11	2.12	0.85
1:A:245:CYS:CA	1:A:276:LEU:HD21	2.06	0.85
1:A:143:TRP:CZ3	1:A:173:PRO:HG2	2.13	0.83
1:A:250:HIS:O	1:A:254:CYS:HB2	1.79	0.83
1:A:168:PHE:CE2	1:A:172:VAL:HG11	2.14	0.83
1:A:71:CYS:HA	1:A:165:ALA:HA	1.62	0.82
1:A:259:CYS:HB3	1:A:262:CYS:CB	2.10	0.80
1:A:227:LYS:HZ3	2:B:53:ASN:HB3	1.46	0.80
1:A:143:TRP:CH2	1:A:173:PRO:CG	2.67	0.77
3:C:103:TYR:CZ	3:C:105:GLY:HA2	2.21	0.75
1:A:143:TRP:HH2	1:A:173:PRO:CG	1.99	0.75
1:A:9:TYR:HD2	1:A:9:TYR:C	1.91	0.74
1:A:259:CYS:CB	1:A:262:CYS:HB2	2.17	0.74
1:A:300:ARG:O	1:A:304:ARG:HG2	1.87	0.74
1:A:9:TYR:HD2	1:A:10:ILE:HD13	1.52	0.74
1:A:9:TYR:CD2	1:A:9:TYR:C	2.62	0.72
1:A:78:LEU:HD13	1:A:139:PRO:HB3	1.72	0.71
1:A:168:PHE:CZ	1:A:172:VAL:HG21	2.24	0.71
1:A:259:CYS:CB	1:A:262:CYS:CB	2.68	0.71
1:A:62:PHE:HE2	1:A:79:PHE:CE2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:OE2	1:A:60:ILE:HD11	1.90	0.70
1:A:138:THR:O	1:A:141:LEU:HG	1.92	0.70
1:A:216:LEU:HD11	1:A:222:ARG:HD3	1.72	0.70
2:B:110:ASP:OD2	2:B:199:LYS:HD3	1.91	0.69
2:B:135:PHE:CE2	3:C:191:SER:HB3	2.26	0.69
1:A:40:VAL:HG13	1:A:121:ALA:HB2	1.75	0.68
1:A:104:ILE:HG22	1:A:112:TYR:HD1	1.56	0.68
1:A:107:ARG:NE	1:A:107:ARG:HA	2.08	0.68
3:C:126:LYS:HA	3:C:126:LYS:HE3	1.74	0.68
1:A:276:LEU:C	1:A:276:LEU:HD23	2.14	0.68
1:A:86:VAL:HG21	1:A:133:PHE:HD1	1.55	0.68
1:A:174:MET:HG2	1:A:257:PHE:HB2	1.76	0.67
3:C:30:THR:HA	3:C:53:PRO:HB2	1.76	0.67
1:A:216:LEU:HB3	1:A:217:PRO:HA	1.77	0.67
3:C:51:ILE:HD13	3:C:72:VAL:HG23	1.78	0.66
1:A:62:PHE:CE2	1:A:79:PHE:CE2	2.78	0.66
2:B:182:THR:HG22	2:B:185:GLU:HB2	1.77	0.66
2:B:94:SER:O	3:C:59:ARG:HD2	1.96	0.66
1:A:17:ALA:O	1:A:21:ILE:HG12	1.96	0.65
1:A:58:LEU:O	1:A:61:PRO:HD2	1.97	0.65
1:A:86:VAL:HG21	1:A:133:PHE:CE1	2.30	0.65
1:A:129:TRP:CD1	5:A:406:STE:H91	2.32	0.64
3:C:60:TYR:HE1	3:C:70:LEU:HG	1.62	0.64
1:A:93:PHE:HB3	1:A:128:CYS:SG	2.38	0.64
3:C:199:TRP:CG	3:C:200:PRO:HA	2.33	0.64
1:A:48:LEU:HD13	1:A:94:SER:HB2	1.80	0.63
1:A:10:ILE:HD11	1:A:64:ILE:CD1	2.28	0.63
1:A:73:ALA:O	1:A:77:CYS:HB2	1.99	0.63
1:A:245:CYS:O	1:A:248:PRO:HD2	1.98	0.63
1:A:111:ARG:O	1:A:115:LEU:HB2	1.99	0.62
1:A:12:VAL:HG12	1:A:13:GLU:N	2.13	0.62
1:A:303:ILE:O	1:A:307:VAL:HB	2.00	0.62
2:B:49:TYR:O	2:B:53:ASN:HB2	2.00	0.62
1:A:70:PHE:CE2	1:A:72:ALA:HB2	2.36	0.61
1:A:10:ILE:HD12	1:A:64:ILE:HG13	1.83	0.61
1:A:246:TRP:CE2	1:A:277:SER:HB2	2.36	0.61
1:A:247:LEU:HD11	5:A:407:STE:H162	1.82	0.61
2:B:27:GLU:O	2:B:69:THR:HG22	1.99	0.61
1:A:290:TYR:OH	5:A:403:STE:H21	2.00	0.61
1:A:32:TRP:NE1	5:A:405:STE:H182	2.16	0.61
1:A:138:THR:N	1:A:139:PRO:HD2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HH22	1:A:233:LYS:HE2	1.65	0.60
1:A:143:TRP:HH2	1:A:173:PRO:CB	2.14	0.60
2:B:33:LEU:HD11	2:B:88:CYS:HB2	1.85	0.59
1:A:182:PHE:HB2	1:A:250:HIS:HD2	1.68	0.59
1:A:264:HIS:CG	1:A:265:ALA:N	2.70	0.59
1:A:10:ILE:CD1	1:A:64:ILE:HD11	2.33	0.59
1:A:57:VAL:HG13	1:A:58:LEU:CD1	2.32	0.59
1:A:107:ARG:HA	1:A:107:ARG:HE	1.67	0.58
1:A:170:ASP:OD1	1:A:170:ASP:N	2.32	0.58
1:A:249:LEU:CB	1:A:273:ALA:HB1	2.31	0.58
2:B:146:VAL:HG21	2:B:175:MET:HE1	1.86	0.58
2:B:94:SER:HB2	3:C:59:ARG:HD3	1.86	0.57
1:A:59:ALA:HB1	1:A:84:VAL:HG12	1.85	0.57
1:A:75:HIS:ND1	1:A:75:HIS:N	2.52	0.57
1:A:70:PHE:CG	1:A:71:CYS:N	2.72	0.57
1:A:289:ALA:O	1:A:296:ARG:HD3	2.05	0.57
1:A:119:THR:O	1:A:122:LYS:HB2	2.05	0.57
1:A:86:VAL:HG23	1:A:132:SER:HB3	1.86	0.56
2:B:182:THR:HG23	2:B:185:GLU:H	1.69	0.56
1:A:32:TRP:HE1	5:A:405:STE:H182	1.71	0.56
3:C:100:GLY:HA3	3:C:110:TYR:CE1	2.41	0.55
1:A:10:ILE:CD1	1:A:64:ILE:CD1	2.84	0.55
1:A:58:LEU:HD23	1:A:83:PHE:CE2	2.42	0.55
1:A:9:TYR:CE2	1:A:13:GLU:HG3	2.42	0.55
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.41	0.55
1:A:57:VAL:CG1	1:A:58:LEU:HD13	2.34	0.54
1:A:307:VAL:HG12	1:A:308:LEU:N	2.22	0.54
1:A:167:LEU:O	1:A:171:VAL:HG13	2.07	0.54
1:A:266:PRO:O	1:A:270:MET:HB3	2.08	0.54
1:A:250:HIS:O	1:A:254:CYS:CB	2.53	0.54
1:A:246:TRP:CD2	1:A:277:SER:HB2	2.43	0.54
1:A:264:HIS:CG	1:A:265:ALA:H	2.25	0.53
1:A:89:GLN:NE2	1:A:185:CYS:HB3	2.23	0.53
5:A:402:STE:H121	6:A:408:LMT:H91	1.90	0.53
1:A:42:ASN:HA	1:A:45:VAL:HB	1.91	0.53
1:A:247:LEU:HB3	1:A:248:PRO:HD3	1.91	0.53
1:A:9:TYR:CD2	1:A:10:ILE:CD1	2.87	0.53
1:A:259:CYS:HG	1:A:262:CYS:HG	1.56	0.53
1:A:174:MET:HE1	1:A:256:THR:HG22	1.91	0.52
1:A:175:ASN:HA	1:A:257:PHE:CZ	2.44	0.52
1:A:205:ARG:HH22	1:A:233:LYS:CE	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:CYS:CA	1:A:276:LEU:CD2	2.85	0.52
1:A:245:CYS:O	1:A:276:LEU:HD22	2.09	0.52
1:A:247:LEU:O	1:A:251:ILE:HG13	2.09	0.52
1:A:274:ILE:HG23	1:A:275:VAL:N	2.25	0.52
1:A:29:TRP:O	1:A:33:LEU:HB2	2.10	0.52
1:A:59:ALA:CB	1:A:84:VAL:HG12	2.39	0.52
1:A:168:PHE:CE1	1:A:172:VAL:HG21	2.44	0.52
1:A:245:CYS:HA	1:A:276:LEU:CD2	2.18	0.52
1:A:267:LEU:O	1:A:271:TYR:HB2	2.10	0.51
1:A:172:VAL:CG1	1:A:172:VAL:O	2.58	0.51
1:A:166:CYS:HA	1:A:171:VAL:HG11	1.92	0.51
1:A:175:ASN:HA	1:A:257:PHE:CE1	2.45	0.51
1:A:10:ILE:HD12	1:A:64:ILE:CG1	2.41	0.51
2:B:184:ASP:O	2:B:188:ARG:HG3	2.11	0.51
1:A:137:LEU:HD13	1:A:140:MET:HB2	1.92	0.51
3:C:199:TRP:CE2	3:C:200:PRO:HB3	2.46	0.50
1:A:120:ARG:O	1:A:124:ILE:HG13	2.11	0.50
1:A:168:PHE:O	1:A:172:VAL:HG12	2.12	0.50
1:A:13:GLU:HB3	1:A:60:ILE:CG1	2.32	0.50
1:A:79:PHE:CD2	1:A:80:ILE:HD12	2.47	0.50
1:A:168:PHE:CE2	4:A:401:ZMA:N16	2.79	0.50
1:A:192:LEU:HA	5:A:402:STE:H101	1.94	0.50
1:A:189:PRO:O	1:A:193:MET:HB2	2.12	0.50
1:A:216:LEU:HA	1:A:218:GLY:H	1.76	0.50
3:C:199:TRP:CD1	3:C:200:PRO:HA	2.47	0.50
1:A:33:LEU:O	1:A:33:LEU:HD22	2.12	0.49
1:A:104:ILE:HG22	1:A:112:TYR:CD1	2.43	0.49
1:A:257:PHE:O	1:A:260:PRO:HD3	2.11	0.49
1:A:130:VAL:HG12	1:A:131:LEU:HD12	1.93	0.49
2:B:205:ILE:H	2:B:205:ILE:HD12	1.77	0.49
1:A:9:TYR:CE1	1:A:271:TYR:CE2	3.00	0.49
1:A:145:ASN:HB2	1:A:173:PRO:HG3	1.93	0.49
3:C:126:LYS:HE3	3:C:127:THR:H	1.77	0.49
1:A:138:THR:OG1	1:A:139:PRO:HD3	2.13	0.49
1:A:193:MET:HA	1:A:196:VAL:HG12	1.93	0.49
3:C:158:PRO:HD2	3:C:212:ALA:CB	2.43	0.49
1:A:52:ASP:HB3	1:A:281:SER:HB3	1.94	0.48
1:A:220:ARG:NH1	1:A:228:GLU:OE2	2.45	0.48
3:C:137:PRO:HD3	3:C:149:LEU:HD23	1.96	0.48
1:A:169:GLU:OE1	1:A:264:HIS:CE1	2.66	0.48
2:B:61:ARG:HH21	2:B:82:ASP:CG	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:LYS:CE	3:C:127:THR:H	2.27	0.48
1:A:129:TRP:NE1	5:A:406:STE:H91	2.28	0.48
1:A:221:ALA:HA	2:B:56:ASP:OD2	2.13	0.48
1:A:66:ILE:HD11	1:A:80:ILE:HG22	1.94	0.48
1:A:79:PHE:HD2	1:A:80:ILE:HD12	1.79	0.48
1:A:167:LEU:O	1:A:171:VAL:HG22	2.13	0.48
1:A:168:PHE:CD2	4:A:401:ZMA:C14	2.97	0.48
2:B:144:ILE:HG22	2:B:163:TRP:CZ3	2.49	0.48
1:A:79:PHE:CD2	1:A:79:PHE:C	2.87	0.48
1:A:82:CYS:HB3	1:A:85:LEU:HG	1.96	0.48
1:A:227:LYS:HZ3	2:B:53:ASN:CB	2.20	0.48
3:C:62:GLN:HA	3:C:65:LYS:HE3	1.95	0.48
1:A:143:TRP:CZ2	1:A:176:TYR:CE2	3.03	0.47
1:A:182:PHE:CD2	1:A:250:HIS:HB3	2.50	0.47
3:C:188:LEU:C	3:C:188:LEU:HD23	2.35	0.47
1:A:60:ILE:HD12	1:A:63:ALA:HB3	1.96	0.47
1:A:182:PHE:O	1:A:187:LEU:HB2	2.14	0.47
2:B:182:THR:CG2	2:B:185:GLU:HB2	2.43	0.47
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.97	0.47
1:A:175:ASN:OD1	1:A:176:TYR:HD2	1.98	0.47
5:A:407:STE:H61	5:A:407:STE:H92	1.46	0.47
1:A:40:VAL:HG21	1:A:116:VAL:HG12	1.94	0.47
1:A:102:ARG:HA	1:A:102:ARG:NE	2.29	0.47
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.62	0.47
2:B:135:PHE:CD2	3:C:191:SER:HB3	2.49	0.47
2:B:193:THR:HG23	7:B:228:HOH:O	2.13	0.47
3:C:163:LEU:C	3:C:163:LEU:HD23	2.35	0.47
1:A:172:VAL:HA	1:A:173:PRO:HD3	1.70	0.47
1:A:16:ILE:HG22	1:A:17:ALA:N	2.29	0.47
1:A:249:LEU:HD21	4:A:401:ZMA:O25	2.15	0.47
1:A:182:PHE:HB2	1:A:250:HIS:CD2	2.50	0.47
2:B:163:TRP:CD1	2:B:163:TRP:N	2.82	0.47
1:A:17:ALA:HB2	1:A:60:ILE:HG21	1.96	0.46
1:A:168:PHE:O	1:A:172:VAL:N	2.41	0.46
1:A:119:THR:HG22	1:A:122:LYS:NZ	2.30	0.46
1:A:307:VAL:CG1	1:A:308:LEU:N	2.78	0.46
1:A:246:TRP:CZ2	1:A:277:SER:HB2	2.51	0.46
2:B:12:SER:HA	2:B:105:GLU:O	2.15	0.46
1:A:290:TYR:HD2	1:A:291:ARG:HG2	1.81	0.46
2:B:4:MET:HE2	2:B:25:ALA:HA	1.97	0.46
2:B:136:LEU:HD21	2:B:196:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:LEU:HB3	3:C:22:CYS:SG	2.55	0.46
1:A:131:LEU:HD12	1:A:131:LEU:N	2.30	0.46
1:A:205:ARG:HH22	1:A:233:LYS:NZ	2.14	0.46
1:A:211:MET:SD	1:A:222:ARG:HG3	2.55	0.46
3:C:129:ALA:HB1	3:C:215:THR:HG21	1.97	0.46
1:A:172:VAL:O	1:A:172:VAL:HG13	2.15	0.46
1:A:187:LEU:O	1:A:191:LEU:HB2	2.15	0.46
1:A:259:CYS:CB	1:A:262:CYS:HB3	2.33	0.46
3:C:35:ASN:OD1	3:C:50:ASN:HB3	2.16	0.46
1:A:9:TYR:HE2	1:A:13:GLU:HG3	1.81	0.46
1:A:251:ILE:O	1:A:254:CYS:HB3	2.16	0.46
1:A:10:ILE:CD1	1:A:64:ILE:HG13	2.45	0.46
1:A:48:LEU:HD13	1:A:94:SER:CB	2.44	0.46
1:A:182:PHE:CE2	1:A:250:HIS:HB3	2.51	0.46
1:A:9:TYR:O	1:A:12:VAL:HB	2.16	0.45
2:B:125:LEU:O	2:B:183:LYS:HD2	2.16	0.45
3:C:18:VAL:O	3:C:82:GLN:HA	2.15	0.45
1:A:86:VAL:HB	1:A:136:GLY:HA3	1.97	0.45
1:A:143:TRP:CZ3	1:A:173:PRO:CG	2.93	0.45
5:A:402:STE:H172	5:A:402:STE:H141	1.69	0.45
1:A:118:GLY:O	1:A:121:ALA:HB3	2.17	0.45
3:C:213:SER:OG	3:C:215:THR:HG23	2.17	0.45
1:A:275:VAL:HG12	1:A:276:LEU:N	2.32	0.45
5:A:403:STE:H122	5:A:403:STE:H152	1.55	0.45
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.99	0.45
1:A:243:ALA:O	1:A:247:LEU:HB2	2.17	0.45
3:C:119:THR:HG22	7:C:259:HOH:O	2.16	0.45
1:A:32:TRP:CE2	5:A:405:STE:H161	2.52	0.45
1:A:19:LEU:HB3	1:A:282:VAL:HG22	1.99	0.44
1:A:264:HIS:CD2	1:A:265:ALA:O	2.70	0.44
2:B:205:ILE:HD12	2:B:205:ILE:N	2.33	0.44
1:A:10:ILE:HD11	1:A:64:ILE:HD11	1.94	0.44
1:A:137:LEU:HD22	1:A:140:MET:HG3	1.99	0.44
1:A:138:THR:N	1:A:139:PRO:CD	2.79	0.44
1:A:60:ILE:HG22	1:A:61:PRO:CD	2.36	0.44
1:A:284:ASN:HB2	1:A:285:PRO:HD3	1.99	0.44
3:C:149:LEU:HD22	3:C:221:ILE:HG21	1.99	0.44
1:A:62:PHE:O	1:A:66:ILE:HG12	2.18	0.44
1:A:89:GLN:HE22	1:A:185:CYS:HB3	1.83	0.44
1:A:178:VAL:HG12	1:A:178:VAL:O	2.18	0.44
1:A:211:MET:SD	1:A:222:ARG:CG	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:C	1:A:276:LEU:CD2	2.86	0.43
2:B:144:ILE:HG22	2:B:163:TRP:HZ3	1.83	0.43
1:A:92:ILE:HD13	1:A:186:VAL:HG22	2.00	0.43
1:A:274:ILE:HG13	1:A:278:HIS:CE1	2.53	0.43
3:C:163:LEU:HA	3:C:207:ASN:O	2.17	0.43
1:A:55:VAL:HG23	1:A:87:LEU:CD1	2.47	0.43
1:A:249:LEU:C	1:A:249:LEU:HD23	2.38	0.43
1:A:175:ASN:O	1:A:179:TYR:HB2	2.17	0.43
1:A:186:VAL:HG12	1:A:187:LEU:N	2.34	0.43
1:A:21:ILE:HD11	1:A:57:VAL:N	2.33	0.43
1:A:51:ALA:HB2	1:A:129:TRP:CH2	2.54	0.43
5:A:405:STE:C15	5:A:405:STE:H92	2.49	0.43
2:B:62:PHE:CE1	2:B:75:ILE:HG12	2.53	0.43
1:A:137:LEU:O	1:A:141:LEU:HD21	2.19	0.43
1:A:216:LEU:HD11	1:A:222:ARG:CD	2.44	0.43
5:A:405:STE:H92	5:A:405:STE:H152	2.00	0.43
2:B:56:ASP:O	2:B:57:ALA:HB3	2.18	0.43
1:A:10:ILE:HD13	1:A:10:ILE:N	2.31	0.43
1:A:62:PHE:HB3	1:A:80:ILE:HG23	2.00	0.43
2:B:124:GLN:HE22	2:B:131:SER:CB	2.32	0.43
1:A:8:VAL:HG13	1:A:9:TYR:N	2.34	0.42
1:A:143:TRP:HZ2	1:A:176:TYR:CE2	2.37	0.42
1:A:23:GLY:O	1:A:26:LEU:HB3	2.20	0.42
1:A:166:CYS:O	1:A:167:LEU:HD12	2.18	0.42
5:A:405:STE:H92	5:A:405:STE:H121	1.81	0.42
2:B:33:LEU:HG	2:B:34:THR:N	2.35	0.42
1:A:6:SER:HB3	1:A:9:TYR:HB3	2.01	0.42
3:C:61:ASN:OD1	3:C:62:GLN:N	2.52	0.42
1:A:34:ASN:OD1	1:A:34:ASN:C	2.56	0.42
3:C:60:TYR:CE1	3:C:70:LEU:HG	2.50	0.42
1:A:28:CYS:CB	5:A:405:STE:H82	2.31	0.42
1:A:245:CYS:SG	1:A:280:ASN:HB2	2.60	0.42
2:B:2:ILE:HG22	2:B:4:MET:CE	2.50	0.42
3:C:126:LYS:HE3	3:C:126:LYS:CA	2.46	0.42
1:A:272:LEU:O	1:A:275:VAL:N	2.53	0.42
5:A:403:STE:H181	5:A:407:STE:H183	2.01	0.42
1:A:129:TRP:CE2	5:A:406:STE:H91	2.55	0.41
2:B:190:ASN:O	2:B:211:ARG:HG3	2.19	0.41
3:C:136:ALA:HB1	3:C:137:PRO:HD2	2.02	0.41
1:A:168:PHE:CE2	4:A:401:ZMA:N17	2.88	0.41
1:A:48:LEU:CD1	1:A:94:SER:HB2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:LYS:HE3	3:C:65:LYS:HB2	1.85	0.41
3:C:129:ALA:CB	3:C:215:THR:HG21	2.50	0.41
2:B:123:GLU:O	2:B:126:THR:HB	2.20	0.41
3:C:38:LYS:HB2	3:C:48:ILE:HD11	2.03	0.41
1:A:29:TRP:HH2	1:A:306:HIS:CD2	2.39	0.41
1:A:60:ILE:HD12	1:A:60:ILE:HA	1.57	0.41
1:A:80:ILE:HD12	1:A:80:ILE:N	2.36	0.41
1:A:119:THR:HA	1:A:122:LYS:HD2	2.03	0.41
5:A:402:STE:H132	5:A:402:STE:H91	2.02	0.41
5:A:403:STE:H31	5:A:404:STE:O2	2.20	0.41
2:B:118:PHE:CD2	2:B:118:PHE:N	2.89	0.41
1:A:9:TYR:CD2	1:A:9:TYR:O	2.74	0.41
2:B:47:LEU:HD12	2:B:47:LEU:HA	1.87	0.41
2:B:59:PRO:HG2	2:B:62:PHE:CD2	2.56	0.41
2:B:147:LYS:HD3	2:B:149:LYS:NZ	2.36	0.41
1:A:9:TYR:CE1	1:A:271:TYR:CD2	3.09	0.40
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.94	0.40
2:B:167:ASP:OD2	2:B:169:LYS:HB3	2.21	0.40
5:A:407:STE:H81	5:A:407:STE:H112	1.69	0.40
2:B:59:PRO:HG2	2:B:62:PHE:HD2	1.86	0.40
1:A:9:TYR:CE2	1:A:13:GLU:CG	3.04	0.40
1:A:143:TRP:NE1	1:A:176:TYR:CZ	2.90	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	293/326 (90%)	259 (88%)	33 (11%)	1 (0%)	41 66
2	B	210/214 (98%)	204 (97%)	6 (3%)	0	100 100
3	C	220/226 (97%)	215 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	723/766 (94%)	678 (94%)	44 (6%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	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	250/276 (91%)	215 (86%)	35 (14%)	3 8
2	B	184/186 (99%)	175 (95%)	9 (5%)	25 52
3	C	193/195 (99%)	182 (94%)	11 (6%)	20 44
All	All	627/657 (95%)	572 (91%)	55 (9%)	10 23

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	10	ILE
1	A	14	LEU
1	A	16	ILE
1	A	18	VAL
1	A	33	LEU
1	A	46	VAL
1	A	57	VAL
1	A	60	ILE
1	A	64	ILE
1	A	75	HIS
1	A	77	CYS
1	A	82	CYS
1	A	84	VAL
1	A	85	LEU

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Mol	Chain	Res	Type
1	A	86	VAL
1	A	92	ILE
1	A	107	ARG
1	A	128	CYS
1	A	137	LEU
1	A	141	LEU
1	A	146	CYS
1	A	170	ASP
1	A	171	VAL
1	A	172	VAL
1	A	191	LEU
1	A	255	PHE
1	A	256	THR
1	A	259	CYS
1	A	262	CYS
1	A	269	LEU
1	A	271	TYR
1	A	279	THR
1	A	282	VAL
1	A	307	VAL
2	B	1	ASP
2	B	17	ASP
2	B	40	GLN
2	B	63	SER
2	B	65	SER
2	B	106	ILE
2	B	107	LYS
2	B	187	GLU
2	B	194	CYS
3	C	30	THR
3	C	41	HIS
3	C	54	TYR
3	C	57	SER
3	C	89	GLU
3	C	126	LYS
3	C	139	CYS
3	C	171	SER
3	C	188	LEU
3	C	214	SER
3	C	215	THR

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

Mol	Chain	Res	Type
1	A	144	ASN
1	A	145	ASN
1	A	250	HIS
1	A	264	HIS

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)

8 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	$\#\|Z\| > 2$
5	STE	A	405	-	19,19,19	0.55	0	19,19,19	0.86	0
5	STE	A	402	-	19,19,19	0.58	0	19,19,19	0.78	0
5	STE	A	404	-	19,19,19	0.58	0	19,19,19	0.82	0
6	LMT	A	408	-	36,36,36	1.45	6 (16%)	47,47,47	1.46	9 (19%)
5	STE	A	406	-	19,19,19	0.53	0	19,19,19	0.99	1 (5%)
4	ZMA	A	401	-	21,28,28	1.66	3 (14%)	20,39,39	1.81	5 (25%)
5	STE	A	403	-	19,19,19	0.56	0	19,19,19	0.89	0
5	STE	A	407	-	19,19,19	0.58	0	19,19,19	0.78	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
5	STE	A	405	-	-	9/17/17/17	-
5	STE	A	402	-	-	11/17/17/17	-
5	STE	A	404	-	-	12/17/17/17	-
6	LMT	A	408	-	-	5/21/61/61	0/2/2/2
5	STE	A	406	-	-	12/17/17/17	-
4	ZMA	A	401	-	-	1/6/10/10	0/4/4/4
5	STE	A	403	-	-	14/17/17/17	-
5	STE	A	407	-	-	12/17/17/17	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ZMA	C11-N10	5.07	1.42	1.34
4	A	401	ZMA	C14-N15	4.51	1.43	1.34
6	A	408	LMT	C3'-C2'	-4.09	1.41	1.52
6	A	408	LMT	C3B-C2B	-4.03	1.42	1.52
6	A	408	LMT	O5B-C1B	2.90	1.49	1.41
6	A	408	LMT	O5'-C1'	2.70	1.48	1.41
6	A	408	LMT	C3'-C4'	-2.46	1.45	1.52
4	A	401	ZMA	C9-N10	-2.10	1.41	1.45
6	A	408	LMT	O5'-C5'	-2.04	1.39	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	ZMA	N12-C11-N13	-3.65	120.46	126.23
4	A	401	ZMA	N15-C14-N16	3.51	120.33	117.97
4	A	401	ZMA	C8-C9-N10	3.42	117.47	111.75
6	A	408	LMT	C1-O1'-C1'	3.39	119.46	113.84
4	A	401	ZMA	C9-N10-C11	-3.09	118.40	123.75
6	A	408	LMT	C1B-O1B-C4'	-3.03	110.45	117.96
6	A	408	LMT	O5'-C1'-C2'	2.93	116.54	110.35
6	A	408	LMT	O1'-C1-C2	2.91	119.76	109.56
6	A	408	LMT	C1'-C2'-C3'	2.47	115.14	110.00
6	A	408	LMT	O3'-C3'-C2'	-2.28	105.07	110.35
6	A	408	LMT	O2'-C2'-C3'	-2.10	105.50	110.35
5	A	406	STE	O2-C1-C2	2.07	120.69	114.03
6	A	408	LMT	O1'-C1'-C2'	2.04	111.49	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	ZMA	N15-C14-N13	2.04	119.71	117.03
6	A	408	LMT	O5B-C5B-C4B	2.00	113.33	109.69

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	STE	C3-C4-C5-C6
5	A	407	STE	C6-C7-C8-C9
5	A	403	STE	C12-C13-C14-C15
5	A	404	STE	C14-C15-C16-C17
5	A	405	STE	C12-C13-C14-C15
5	A	407	STE	C11-C10-C9-C8
5	A	406	STE	C12-C13-C14-C15
5	A	405	STE	C9-C10-C11-C12
6	A	408	LMT	O5'-C5'-C6'-O6'
5	A	407	STE	C12-C13-C14-C15
6	A	408	LMT	C2'-C1'-O1'-C1
5	A	402	STE	C14-C15-C16-C17
5	A	406	STE	C11-C10-C9-C8
6	A	408	LMT	C4'-C5'-C6'-O6'
5	A	404	STE	C1-C2-C3-C4
5	A	405	STE	C11-C12-C13-C14
5	A	402	STE	C9-C10-C11-C12
5	A	407	STE	C7-C8-C9-C10
5	A	403	STE	C10-C11-C12-C13
5	A	406	STE	C4-C5-C6-C7
5	A	404	STE	C10-C11-C12-C13
5	A	405	STE	C11-C10-C9-C8
5	A	402	STE	C13-C14-C15-C16
5	A	405	STE	C5-C6-C7-C8
5	A	406	STE	C7-C8-C9-C10
6	A	408	LMT	C4-C5-C6-C7
5	A	403	STE	C14-C15-C16-C17
5	A	407	STE	C4-C5-C6-C7
5	A	402	STE	C1-C2-C3-C4
5	A	403	STE	C11-C12-C13-C14
5	A	403	STE	C9-C10-C11-C12
5	A	404	STE	C13-C14-C15-C16
5	A	405	STE	C7-C8-C9-C10
5	A	405	STE	C2-C3-C4-C5
5	A	404	STE	C6-C7-C8-C9

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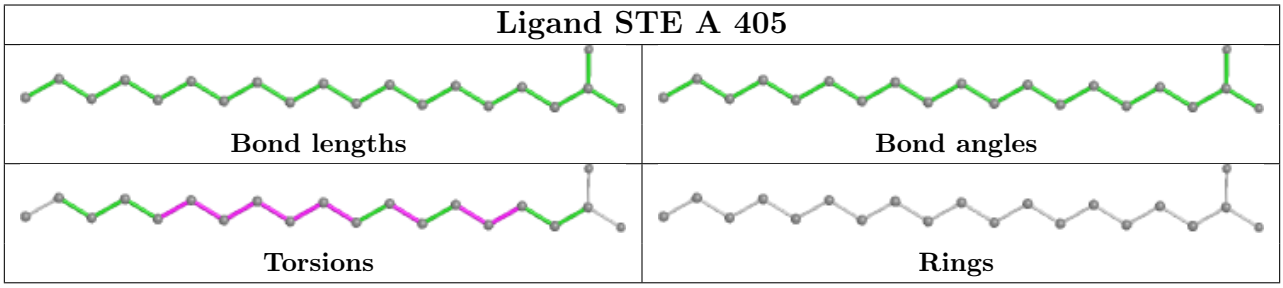
Mol	Chain	Res	Type	Atoms
5	A	404	STE	C9-C10-C11-C12
6	A	408	LMT	C5-C6-C7-C8
5	A	406	STE	C2-C3-C4-C5
5	A	407	STE	C5-C6-C7-C8
5	A	403	STE	C13-C14-C15-C16
5	A	407	STE	C9-C10-C11-C12
5	A	402	STE	C11-C10-C9-C8
5	A	406	STE	C1-C2-C3-C4
5	A	404	STE	C11-C12-C13-C14
5	A	402	STE	C10-C11-C12-C13
5	A	403	STE	C15-C16-C17-C18
5	A	403	STE	C2-C3-C4-C5
5	A	404	STE	C7-C8-C9-C10
5	A	405	STE	C10-C11-C12-C13
5	A	403	STE	C3-C4-C5-C6
5	A	406	STE	C5-C6-C7-C8
5	A	406	STE	C6-C7-C8-C9
5	A	407	STE	C10-C11-C12-C13
5	A	402	STE	C11-C12-C13-C14
5	A	404	STE	C3-C4-C5-C6
5	A	403	STE	C11-C10-C9-C8
5	A	403	STE	C7-C8-C9-C10
5	A	402	STE	C12-C13-C14-C15
5	A	407	STE	C14-C15-C16-C17
5	A	405	STE	C3-C4-C5-C6
5	A	403	STE	C5-C6-C7-C8
4	A	401	ZMA	C8-C9-N10-C11
5	A	402	STE	O2-C1-C2-C3
5	A	404	STE	O1-C1-C2-C3
5	A	402	STE	C6-C7-C8-C9
5	A	403	STE	O2-C1-C2-C3
5	A	402	STE	O1-C1-C2-C3
5	A	403	STE	O1-C1-C2-C3
5	A	404	STE	O2-C1-C2-C3
5	A	406	STE	C15-C16-C17-C18
5	A	407	STE	O2-C1-C2-C3
5	A	406	STE	O2-C1-C2-C3
5	A	407	STE	O1-C1-C2-C3
5	A	404	STE	C15-C16-C17-C18
5	A	406	STE	O1-C1-C2-C3
5	A	407	STE	C15-C16-C17-C18

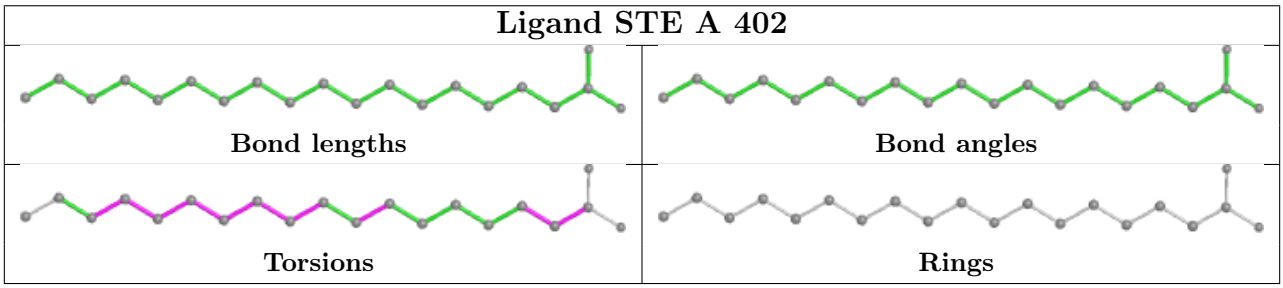
There are no ring outliers.

8 monomers are involved in 26 short contacts:

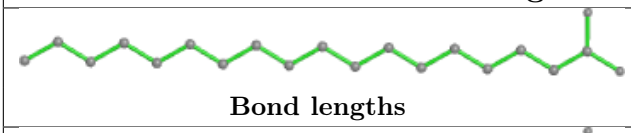
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	STE	8	0
5	A	402	STE	4	0
5	A	404	STE	1	0
6	A	408	LMT	1	0
5	A	406	STE	3	0
4	A	401	ZMA	4	0
5	A	403	STE	4	0
5	A	407	STE	4	0

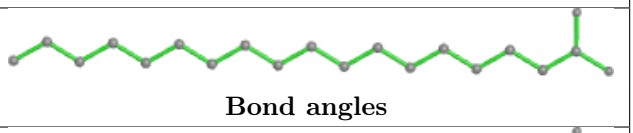
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

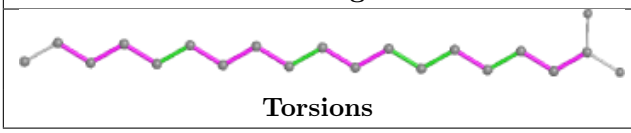


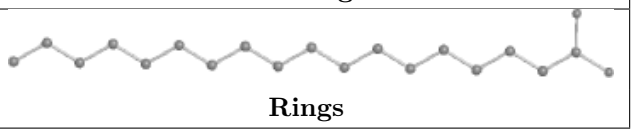


Ligand STE A 404

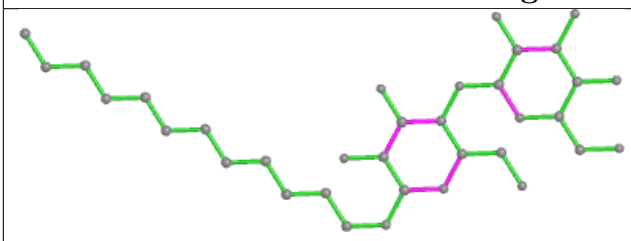

Bond lengths

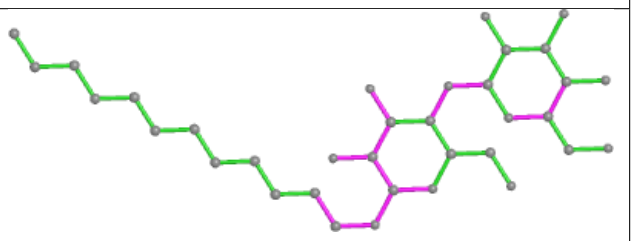

Bond angles

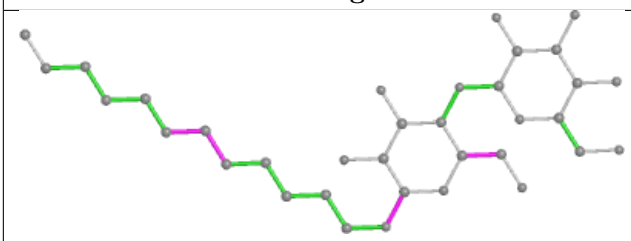

Torsions

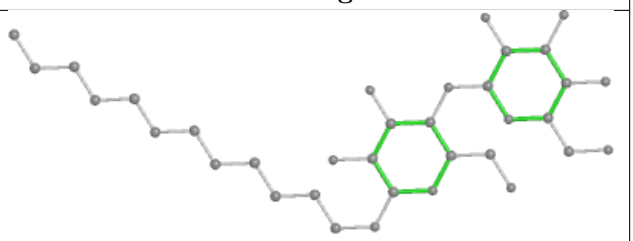

Rings

Ligand LMT A 408

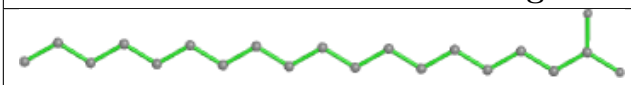

Bond lengths

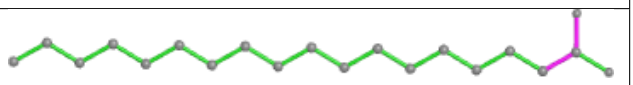

Bond angles

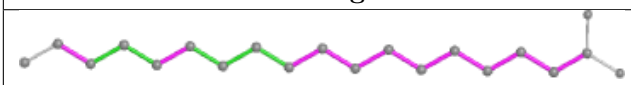

Torsions

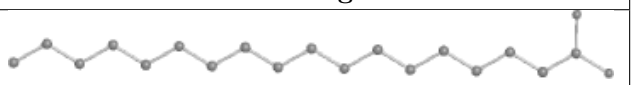

Rings

Ligand STE A 406

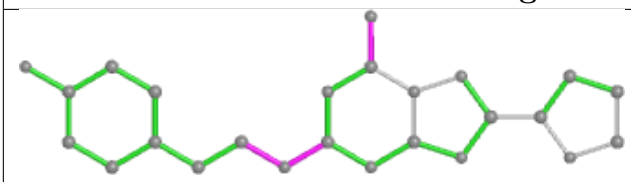

Bond lengths

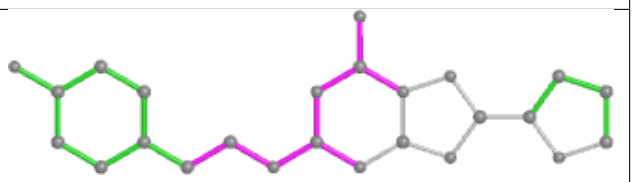

Bond angles

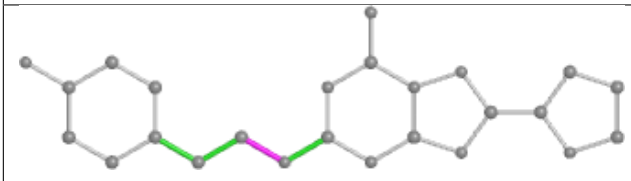

Torsions

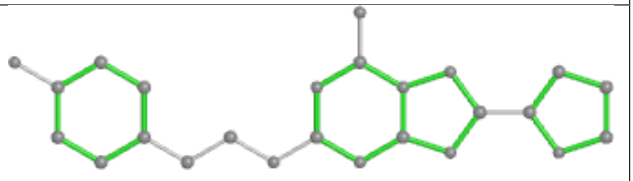

Rings

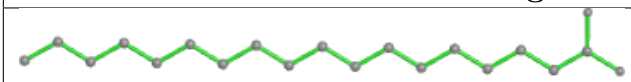
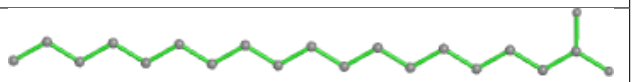
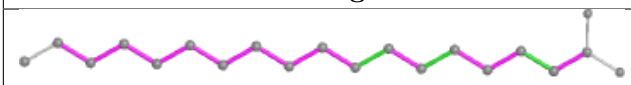
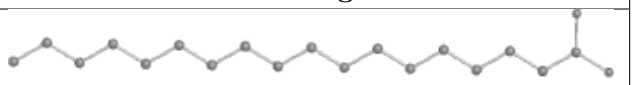
Ligand ZMA A 401

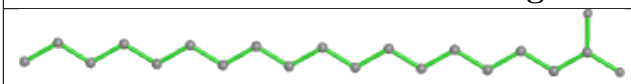
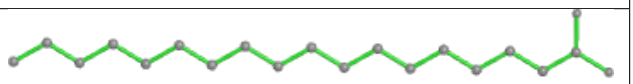
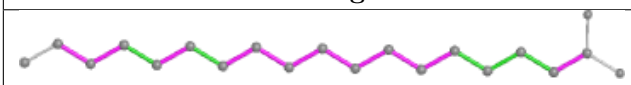
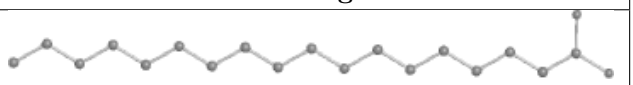

Bond lengths


Bond angles


Torsions


Rings

Ligand STE A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	297/326 (91%)	0.73	50 (16%) 1 1	59, 112, 181, 205	0
2	B	212/214 (99%)	0.08	4 (1%) 66 69	41, 61, 99, 145	0
3	C	224/226 (99%)	0.13	2 (0%) 84 85	39, 60, 101, 150	0
All	All	733/766 (95%)	0.36	56 (7%) 13 12	39, 76, 164, 205	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	7.2
1	A	142	GLY	7.2
1	A	78	LEU	6.9
1	A	268	TRP	6.7
1	A	261	ASP	6.1
1	A	84	VAL	4.9
1	A	246	TRP	4.8
1	A	82	CYS	4.4
1	A	271	TYR	4.3
1	A	77	CYS	4.3
1	A	79	PHE	4.1
1	A	259	CYS	4.0
1	A	267	LEU	3.9
1	A	80	ILE	3.5
1	A	140	MET	3.5
1	A	262	CYS	3.4
1	A	242	PHE	3.4
2	B	187	GLU	3.4
1	A	275	VAL	3.3
1	A	162	GLY	3.2
1	A	168	PHE	3.2
1	A	74	CYS	3.2
1	A	263	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	144	ASN	3.1
1	A	273	ALA	3.0
1	A	83	PHE	3.0
1	A	66	ILE	2.9
1	A	141	LEU	2.9
1	A	161	GLU	2.8
1	A	158	GLY	2.7
1	A	137	LEU	2.7
1	A	279	THR	2.7
3	C	225	GLY	2.7
1	A	177	MET	2.6
2	B	188	ARG	2.6
2	B	152	GLY	2.6
1	A	8	VAL	2.6
1	A	55	VAL	2.6
1	A	309	ARG	2.5
1	A	217	PRO	2.5
1	A	86	VAL	2.5
1	A	258	PHE	2.5
1	A	147	GLY	2.4
1	A	280	ASN	2.3
1	A	172	VAL	2.3
1	A	239	VAL	2.3
1	A	190	LEU	2.3
1	A	146	CYS	2.3
1	A	216	LEU	2.2
3	C	226	PRO	2.2
1	A	76	GLY	2.1
1	A	252	ILE	2.1
2	B	155	ARG	2.1
1	A	65	THR	2.1
1	A	59	ALA	2.0
1	A	264	HIS	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

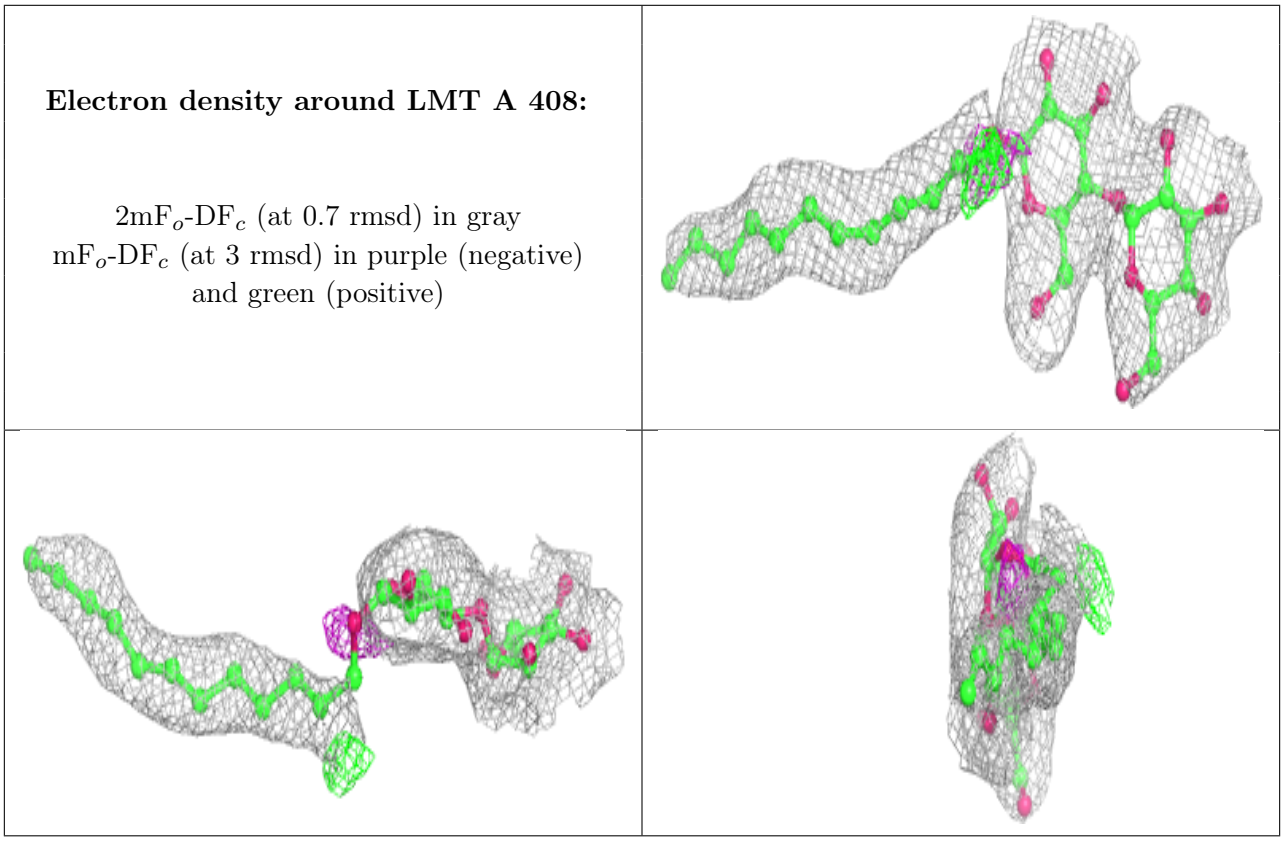
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	LMT	A	408	35/35	0.66	0.18	92,139,157,158	0
5	STE	A	405	20/20	0.68	0.40	101,116,139,140	0
5	STE	A	402	20/20	0.68	0.53	113,126,140,142	0
5	STE	A	406	20/20	0.71	0.29	110,118,136,138	0
5	STE	A	403	20/20	0.76	0.23	95,108,166,167	0
5	STE	A	407	20/20	0.79	0.46	114,121,129,130	0
4	ZMA	A	401	25/25	0.80	0.42	149,163,194,198	0
5	STE	A	404	20/20	0.80	0.28	88,110,126,127	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.

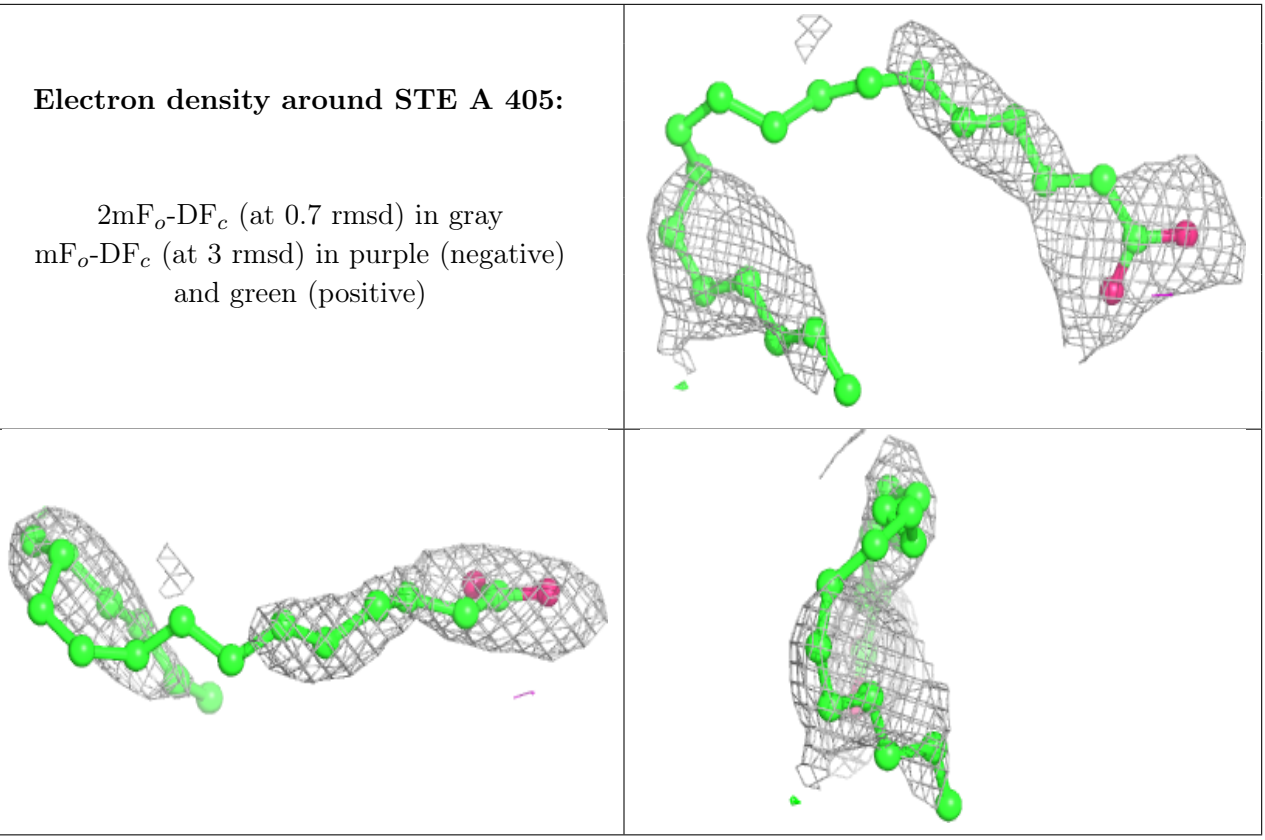
Electron density around LMT A 408:

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



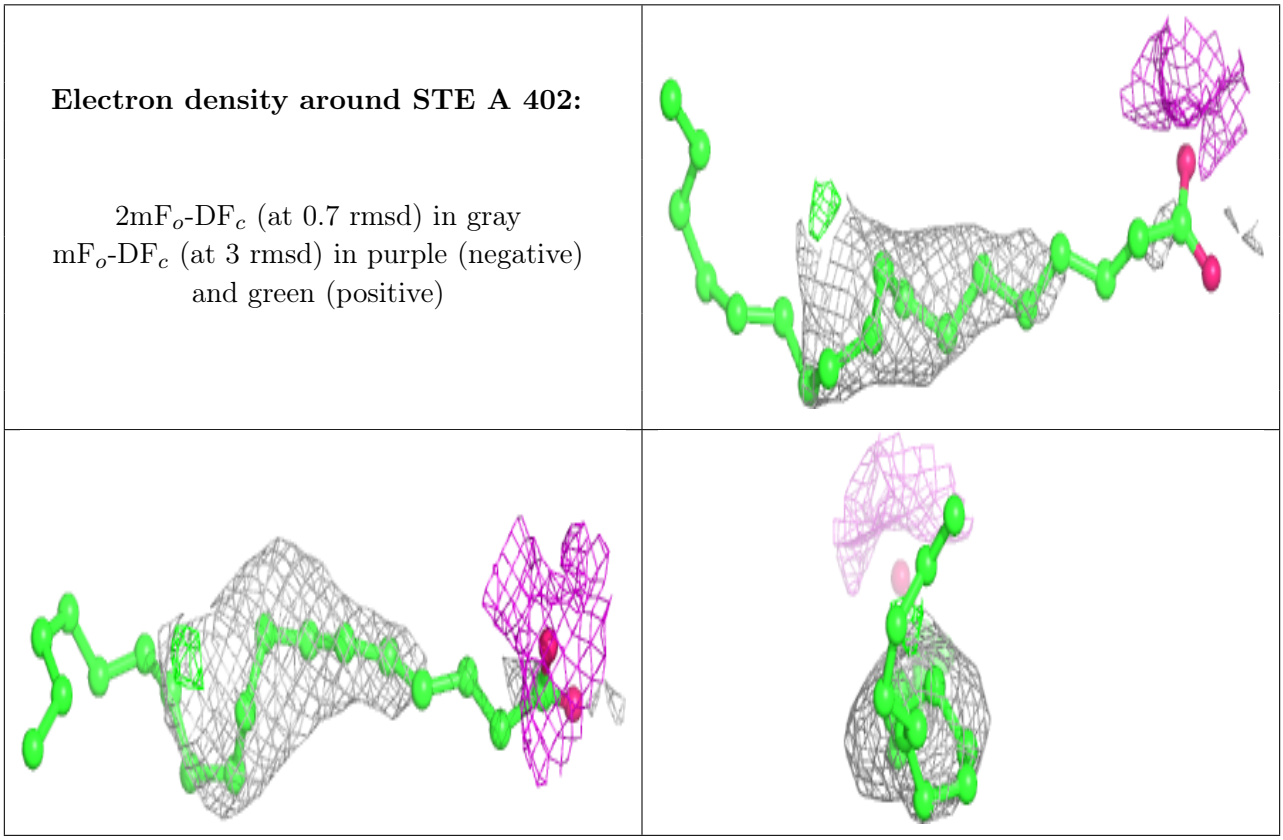
Electron density around STE A 405:

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



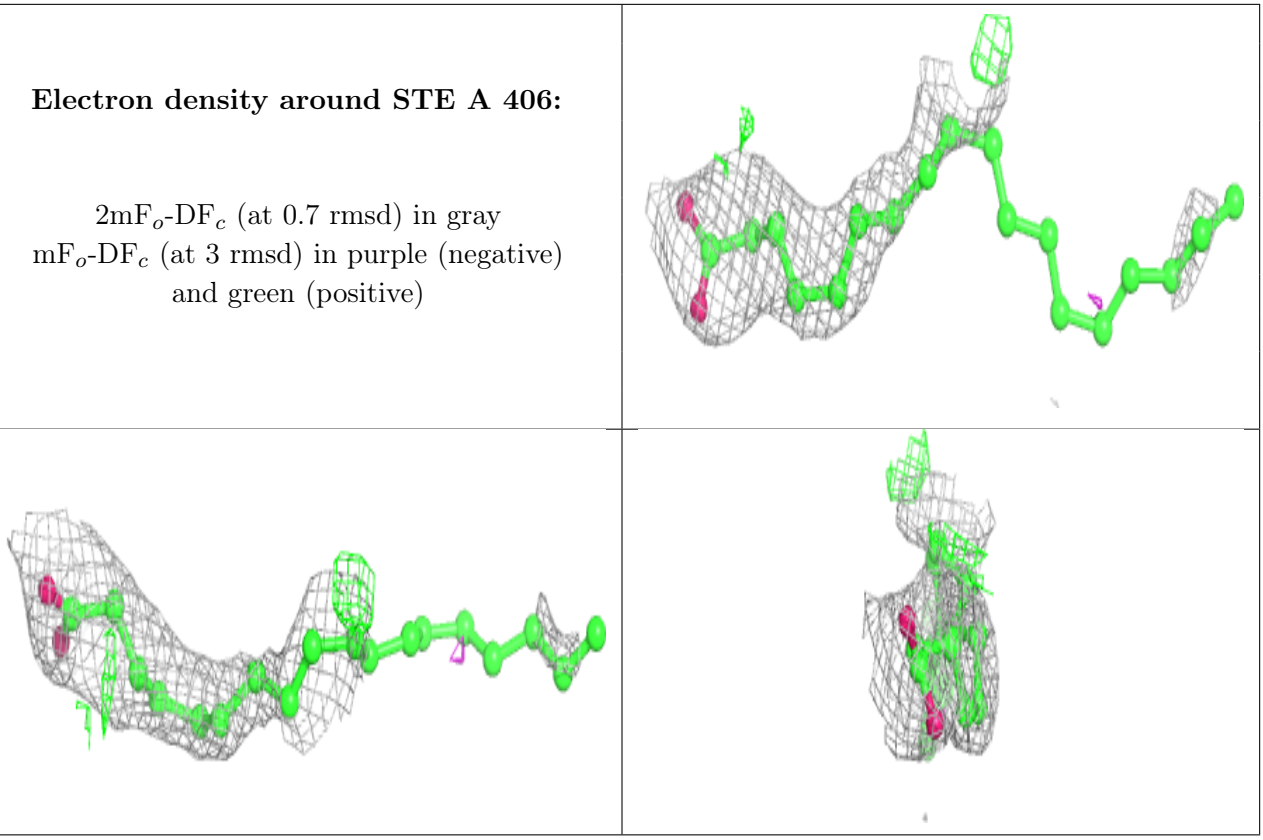
Electron density around STE A 402:

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



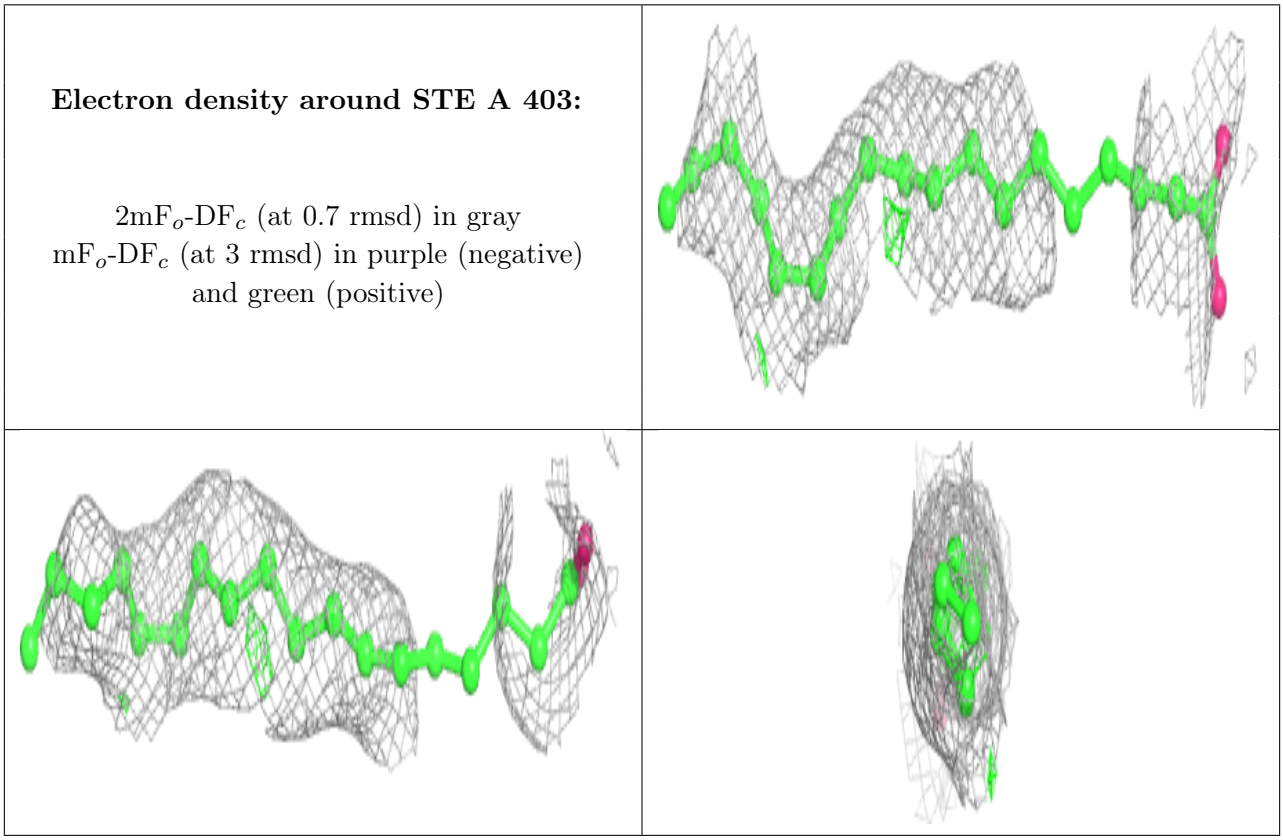
Electron density around STE A 406:

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



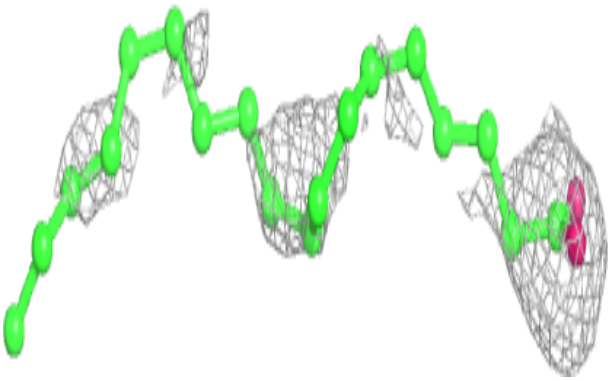
Electron density around STE A 403:

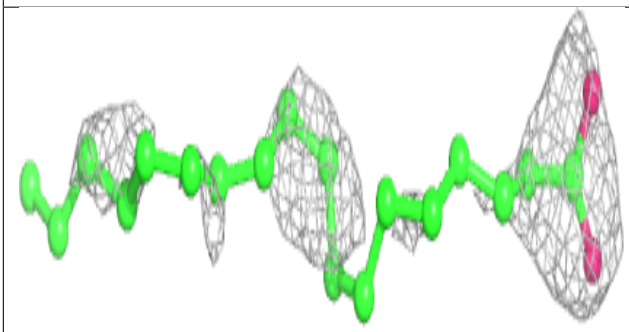
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

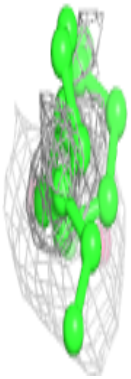


Electron density around STE A 407:

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

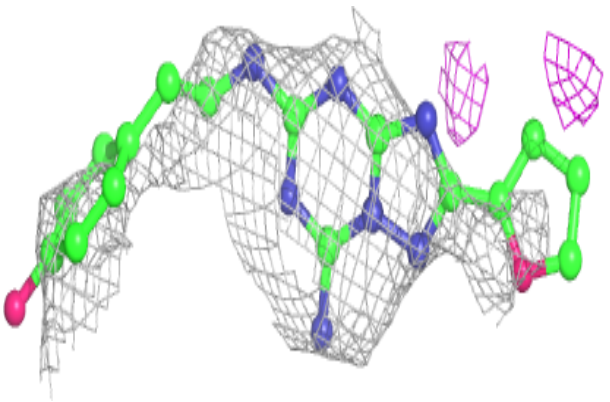


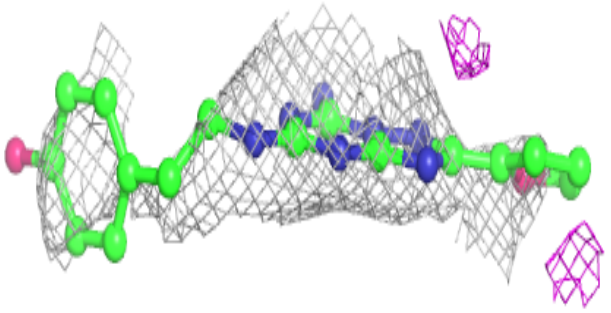


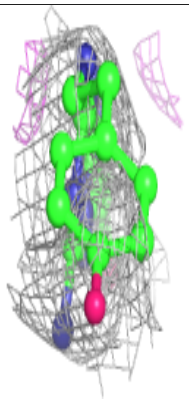


Electron density around ZMA A 401:

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

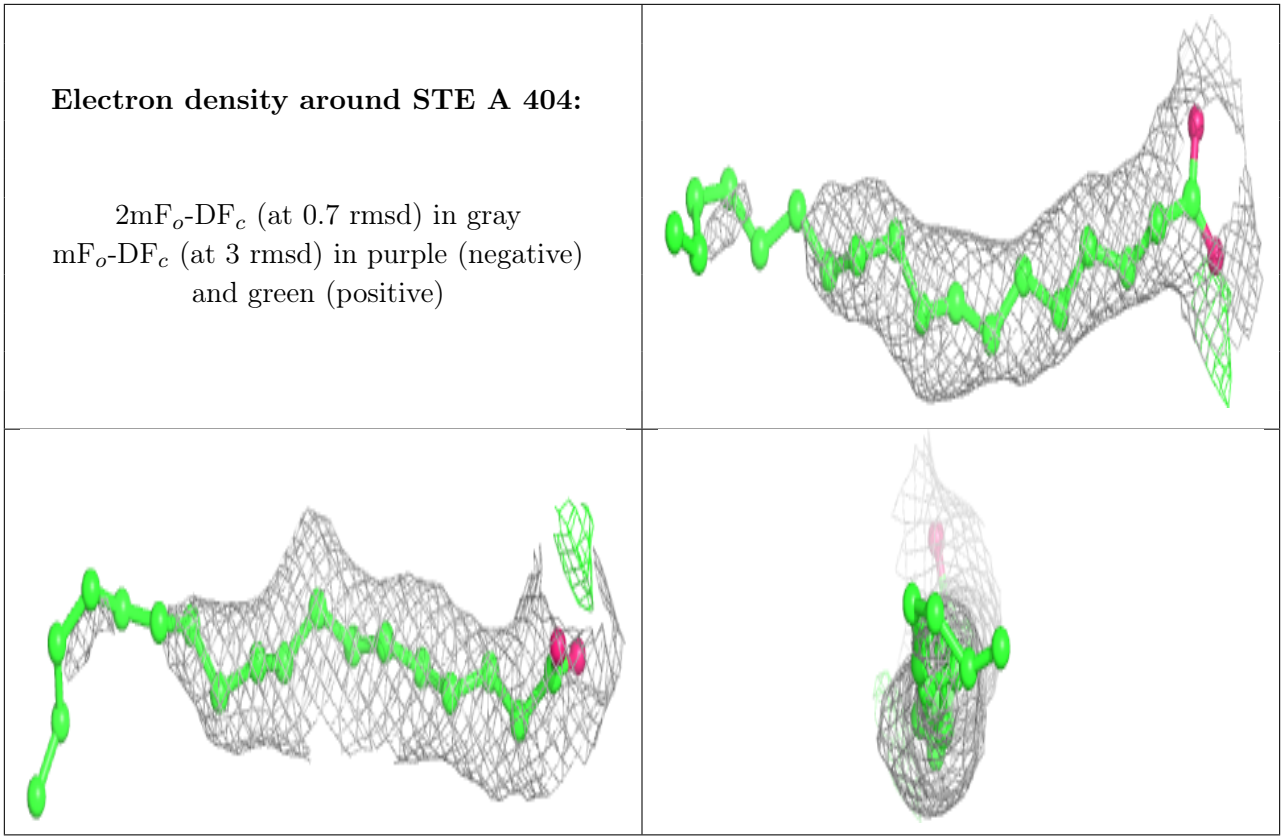






Electron density around STE A 404:

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



6.5 Other polymers (i)

There are no such residues in this entry.