



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:11 AM UTC

PDB ID : 3VG9 / pdb_00003vg9
Title : Crystal structure of human adenosine A2A receptor with an allosteric inverse-agonist antibody at 2.7 Å 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

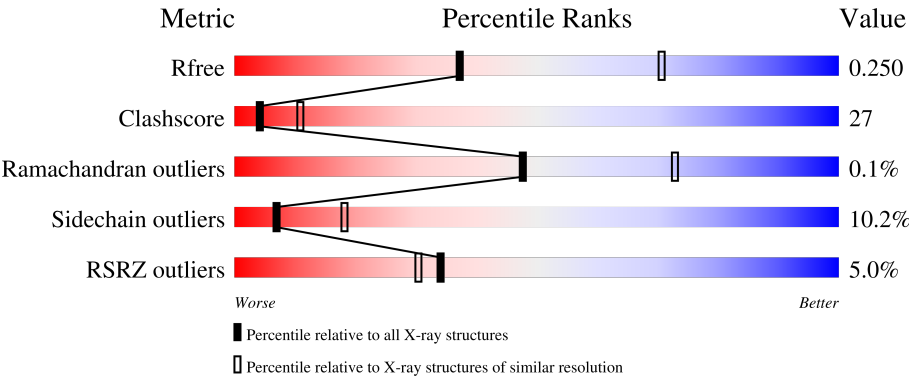
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	9% 40% 41% 10% 9%
2	B	214	2% 68% 31%
3	C	226	% 77% 20%

2 Entry composition

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
1	A	297	Total	C	N	O	S	0	0	0
			2318	1529	388	381	20			

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

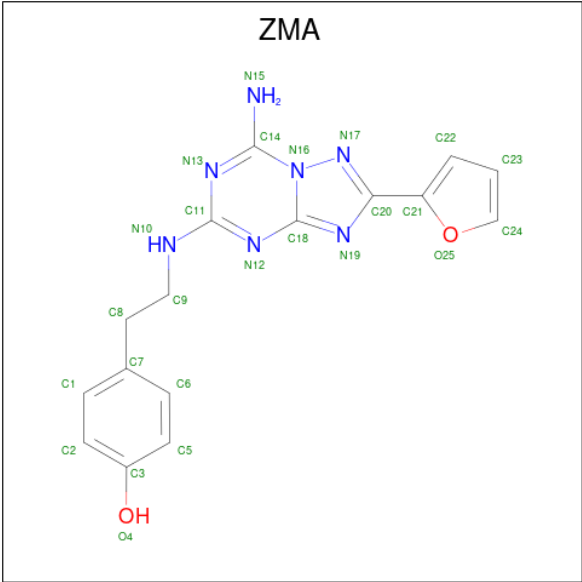
- Molecule 2 is a protein called antibody fab fragment light chain.

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

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

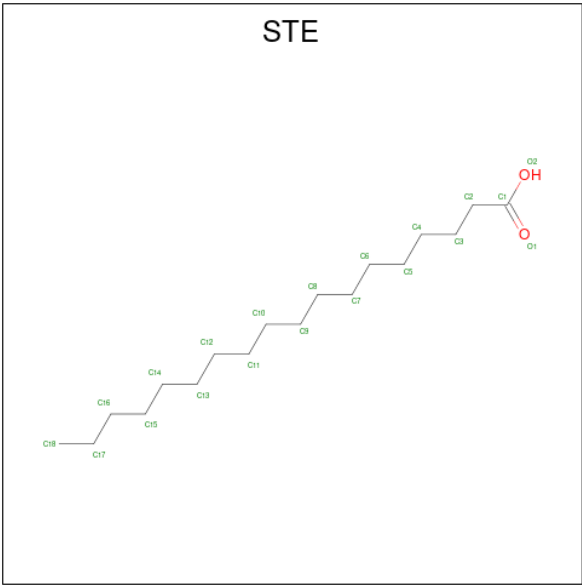
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	224	Total	C	N	O	S	0	0	0
			1694	1067	279	342	6			

- 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 (CCD ID: ZMA) (formula: C₁₆H₁₅N₇O₂).



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

- Molecule 5 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



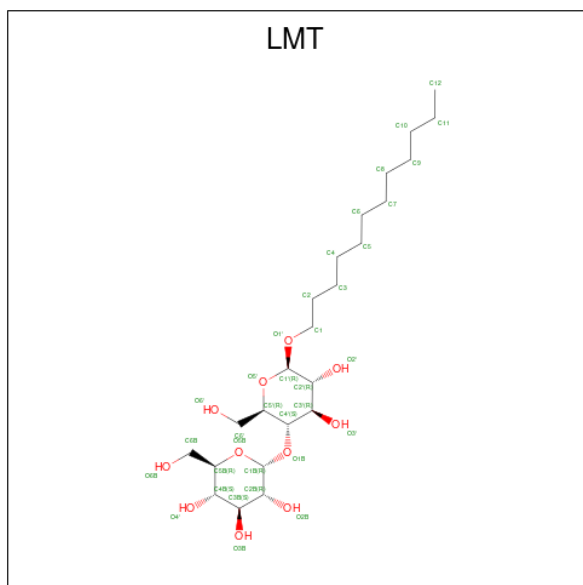
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	18	2		
5	A	1	Total	C	O	0	0
			20	18	2		
5	A	1	Total	C	O	0	0
			20	18	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	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		

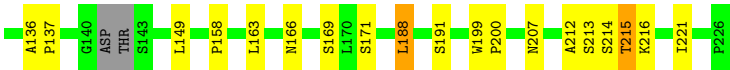
- Molecule 6 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 7 is water.

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



4 Data and refinement statistics

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 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-2.70) 92.4 (20.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 0.250	Depositor DCC
R_{free} test set	2114 reflections (4.67%)	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)	0.28 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/2374	0.84	6/3236 (0.2%)
2	B	0.43	0/1678	0.84	0/2280
3	C	0.41	0/1736	0.80	0/2366
All	All	0.41	0/5788	0.83	6/7882 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ASN	N-CA-C	6.72	119.36	108.34
1	A	265	ALA	CA-C-N	5.60	126.84	119.84
1	A	265	ALA	C-N-CA	5.60	126.84	119.84
1	A	72	ALA	N-CA-C	5.57	115.19	107.73
1	A	172	VAL	CA-C-N	5.53	125.70	119.90
1	A	172	VAL	C-N-CA	5.53	125.70	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2318	0	2393	229	0
2	B	1639	0	1562	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1694	0	1640	37	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	318	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 27.

All (318) 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:9:TYR:HD2	1:A:9:TYR:C	1.91	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TRP:CH2	1:A:173:PRO:CG	2.67	0.77
1:A:9:TYR:CD2	1:A:9:TYR:C	2.62	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: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:276:LEU:C	1:A:276:LEU:HD23	2.14	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
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:86:VAL:HG21	1:A:133:PHE:HD1	1.55	0.68
2:B:161:ASN:HB3	2:B:175:MET:HE3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2:ILE:HG22	2:B:4:MET:HE3	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
1:A:190:LEU:HA	1:A:193:MET:HE2	1.87	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:O	1:A:270:MET:HB3	2.08	0.54
2:B:175:MET:HE2	2:B:177:SER:HB2	1.89	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
2:B:61:ARG:HH21	2:B:82:ASP:CG	2.16	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:174:MET:HE3	1:A:257:PHE:HA	1.90	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:79:PHE:C	1:A:79:PHE:CD2	2.87	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
3:C:188:LEU:C	3:C:188:LEU:HD23	2.35	0.52
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
2:B:4:MET:HE1	2:B:25:ALA:CB	2.41	0.52
1:A:267:LEU:O	1:A:271:TYR:HB2	2.10	0.51
3:C:163:LEU:C	3:C:163:LEU:HD23	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:249:LEU:C	1:A:249:LEU:HD23	2.38	0.49
2:B:3:VAL:C	2:B:4:MET:HE2	2.38	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
1:A:276:LEU:C	1:A:276:LEU:CD2	2.86	0.48
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:34:ASN:C	1:A:34:ASN:OD1	2.56	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:136:LEU:HD21	2:B:196:ALA:HB2	1.98	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:LEU:C	1:A:61:PRO:HD2	2.41	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
2:B:17:ASP:OD1	2:B:17:ASP:C	2.61	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
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: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
3:C:40:SER:C	3:C:41:HIS:CG	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:83:PHE:C	1:A:85:LEU:N	2.76	0.42
2:B:4:MET:HE1	2:B:25:ALA:HB1	2.02	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:193:MET:HE3	1:A:239:VAL:CG1	2.50	0.41
2:B:161:ASN:CB	2:B:175:MET:HE3	2.44	0.41
1:A:48:LEU:CD1	1:A:94:SER:HB2	2.47	0.41
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:166:ASN:HB3	3:C:169:SER:HG	1.86	0.41
1:A:113:ASN:OD1	1:A:113:ASN:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:407:STE:H81	5:A:407:STE:H112	1.69	0.40
2:B:2:ILE:HG22	2:B:4:MET:CE	2.50	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%)	36	60
2	B	210/214 (98%)	204 (97%)	6 (3%)	0	100	100
3	C	220/226 (97%)	215 (98%)	5 (2%)	0	100	100
All	All	723/766 (94%)	678 (94%)	44 (6%)	1 (0%)	48	73

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%)	209 (84%)	41 (16%)	2	6
2	B	184/186 (99%)	172 (94%)	12 (6%)	15	37
3	C	193/195 (99%)	182 (94%)	11 (6%)	18	43
All	All	627/657 (95%)	563 (90%)	64 (10%)	7	18

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	10	ILE
1	A	12	VAL
1	A	14	LEU
1	A	16	ILE
1	A	18	VAL
1	A	25	VAL
1	A	33	LEU
1	A	46	VAL
1	A	48	LEU
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
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	220	ARG
1	A	255	PHE
1	A	256	THR
1	A	259	CYS
1	A	262	CYS

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	271	TYR
1	A	272	LEU
1	A	275	VAL
1	A	279	THR
1	A	282	VAL
1	A	307	VAL
2	B	1	ASP
2	B	14	SER
2	B	40	GLN
2	B	63	SER
2	B	65	SER
2	B	76	ASN
2	B	106	ILE
2	B	107	LYS
2	B	156	GLN
2	B	160	LEU
2	B	187	GLU
2	B	194	CYS
3	C	20	ILE
3	C	30	THR
3	C	41	HIS
3	C	57	SER
3	C	89	GLU
3	C	126	LYS
3	C	171	SER
3	C	188	LEU
3	C	214	SER
3	C	215	THR
3	C	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	89	GLN
1	A	145	ASN
1	A	250	HIS
1	A	264	HIS
2	B	38	GLN
2	B	76	ASN
2	B	210	ASN

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Mol	Chain	Res	Type
3	C	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	407	-	19,19,19	0.63	0	19,19,19	0.79	0
5	STE	A	402	-	19,19,19	0.64	0	19,19,19	0.78	0
6	LMT	A	408	-	36,36,36	1.44	6 (16%)	47,47,47	1.48	9 (19%)
5	STE	A	405	-	19,19,19	0.60	0	19,19,19	0.87	0
4	ZMA	A	401	-	26,28,28	1.67	4 (15%)	30,39,39	2.38	7 (23%)
5	STE	A	404	-	19,19,19	0.63	0	19,19,19	0.83	0
5	STE	A	406	-	19,19,19	0.58	0	19,19,19	1.00	1 (5%)
5	STE	A	403	-	19,19,19	0.61	0	19,19,19	0.90	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	407	-	-	12/17/17/17	-
5	STE	A	402	-	-	11/17/17/17	-
6	LMT	A	408	-	-	5/21/61/61	0/2/2/2
5	STE	A	405	-	-	9/17/17/17	-
4	ZMA	A	401	-	-	1/10/10/10	0/4/4/4
5	STE	A	404	-	-	12/17/17/17	-
5	STE	A	406	-	-	12/17/17/17	-
5	STE	A	403	-	-	14/17/17/17	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ZMA	C14-N15	5.36	1.43	1.34
6	A	408	LMT	C3'-C2'	-4.02	1.41	1.52
6	A	408	LMT	C3B-C2B	-3.96	1.42	1.52
4	A	401	ZMA	C18-N16	-3.45	1.33	1.38
4	A	401	ZMA	C18-N19	3.20	1.38	1.33
6	A	408	LMT	O5B-C1B	2.88	1.49	1.41
6	A	408	LMT	O5'-C1'	2.68	1.48	1.41
6	A	408	LMT	C3'-C4'	-2.40	1.45	1.52
4	A	401	ZMA	C9-N10	-2.05	1.41	1.46
6	A	408	LMT	O5'-C5'	-2.04	1.39	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ZMA	N17-C20-N19	-6.78	107.72	115.38
4	A	401	ZMA	C20-N17-N16	6.33	107.94	101.39
4	A	401	ZMA	C18-N16-N17	-3.83	107.56	110.41
4	A	401	ZMA	N13-C11-N12	-3.65	120.46	126.79
6	A	408	LMT	C1-O1'-C1'	3.38	119.46	113.68
4	A	401	ZMA	N16-C18-N12	-3.31	119.73	122.61
6	A	408	LMT	C1B-O1B-C4'	-3.17	110.45	117.98
6	A	408	LMT	O1'-C1-C2	3.06	119.76	109.37
6	A	408	LMT	O5'-C1'-C2'	3.00	116.54	110.37
4	A	401	ZMA	N10-C11-N12	2.97	119.97	116.95
4	A	401	ZMA	N12-C18-N19	2.92	132.35	127.73
6	A	408	LMT	C1'-C2'-C3'	2.44	115.14	110.01
6	A	408	LMT	O3'-C3'-C2'	-2.25	105.07	110.38
6	A	408	LMT	O1'-C1'-C2'	2.12	111.49	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	STE	O2-C1-C2	2.12	120.69	114.00
6	A	408	LMT	O2'-C2'-C3'	-2.07	105.50	110.38
6	A	408	LMT	O5B-C5B-C4B	2.02	113.33	109.70

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

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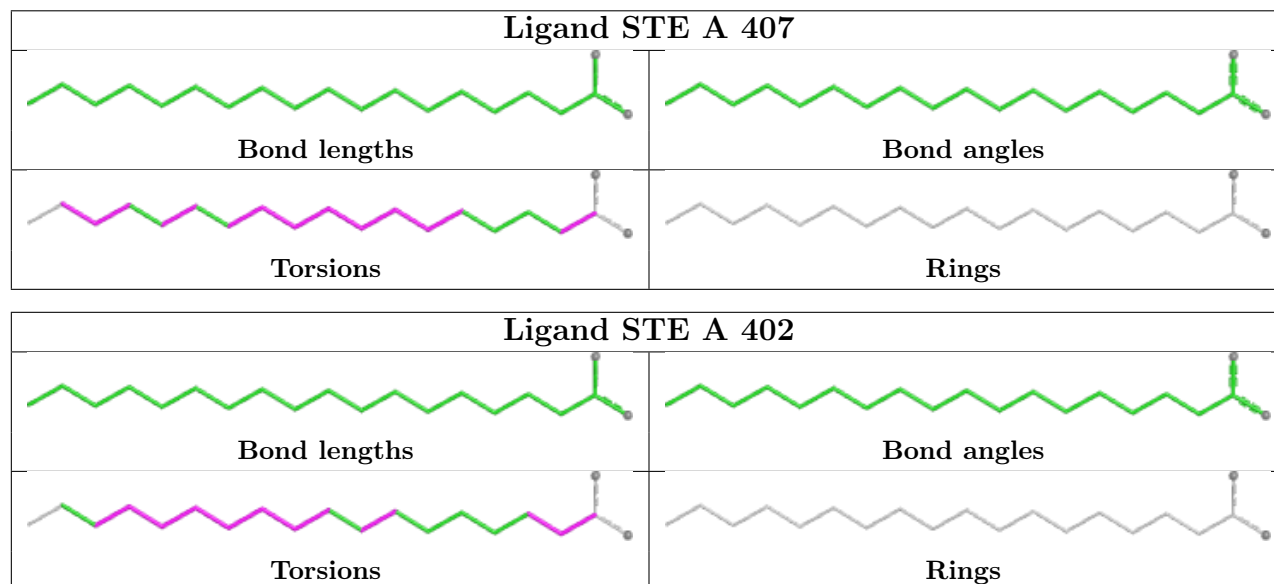
Mol	Chain	Res	Type	Atoms
5	A	405	STE	C2-C3-C4-C5
5	A	404	STE	C6-C7-C8-C9
5	A	402	STE	C11-C10-C9-C8
6	A	408	LMT	C5-C6-C7-C8
5	A	402	STE	C10-C11-C12-C13
5	A	406	STE	C2-C3-C4-C5
5	A	403	STE	C13-C14-C15-C16
5	A	407	STE	C5-C6-C7-C8
5	A	407	STE	C9-C10-C11-C12
5	A	406	STE	C1-C2-C3-C4
5	A	404	STE	C11-C12-C13-C14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

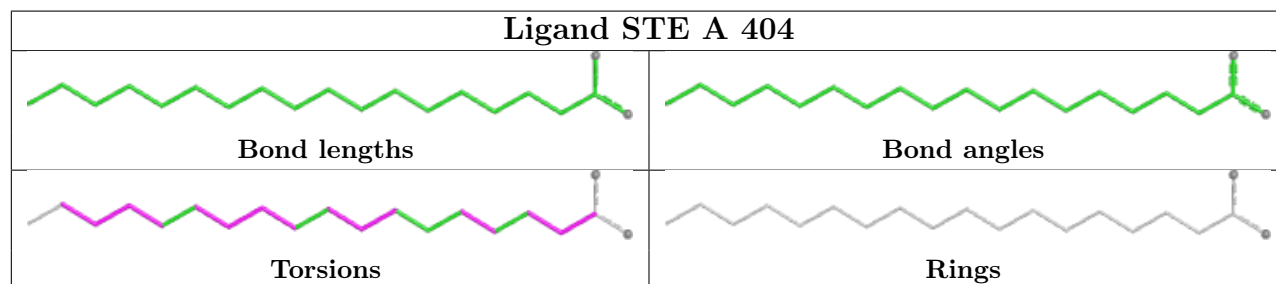
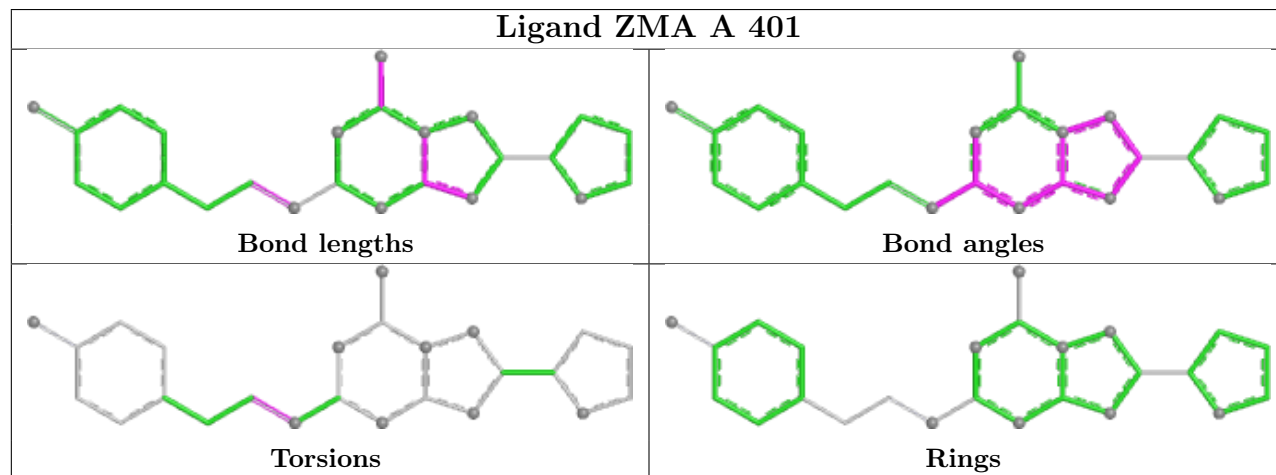
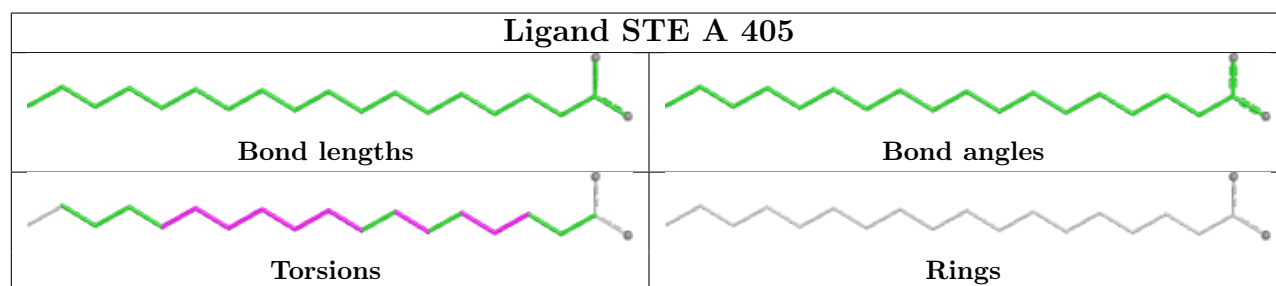
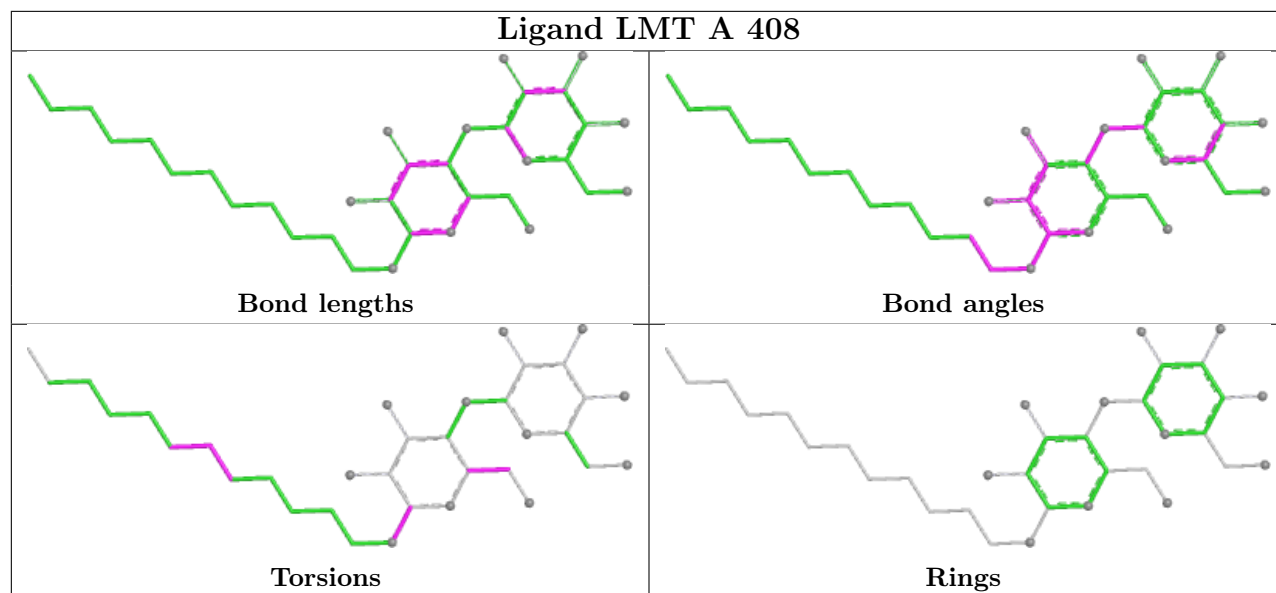
There are no ring outliers.

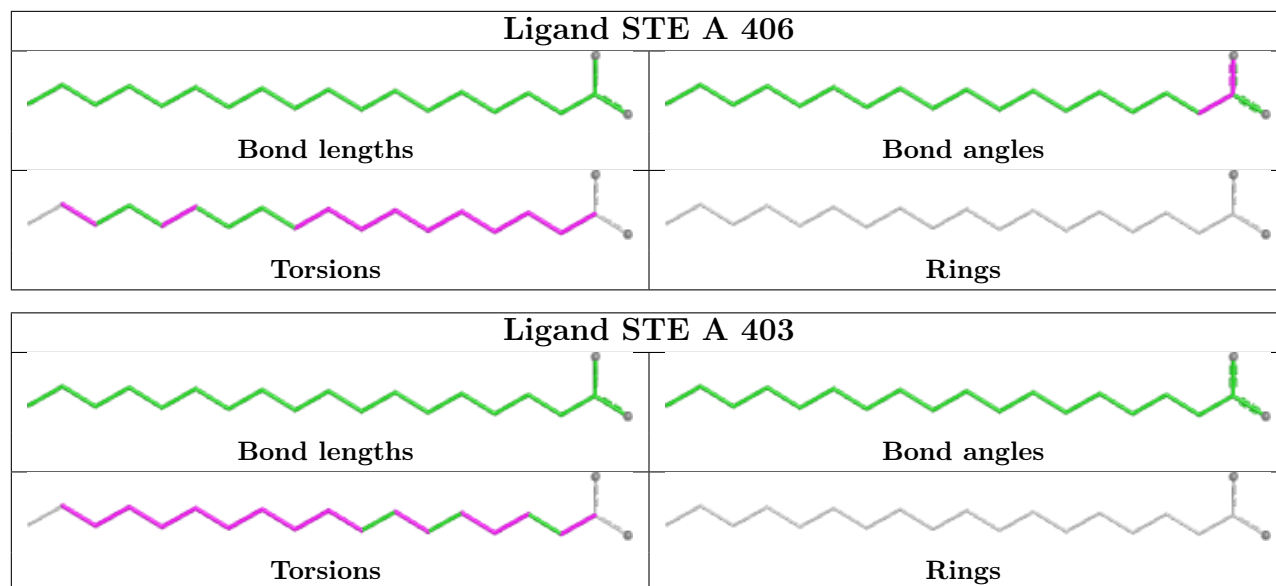
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	STE	4	0
5	A	402	STE	4	0
6	A	408	LMT	1	0
5	A	405	STE	8	0
4	A	401	ZMA	4	0
5	A	404	STE	1	0
5	A	406	STE	3	0
5	A	403	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/326 (91%)	0.67	30 (10%) 12 10	59, 112, 181, 205	0
2	B	212/214 (99%)	0.02	5 (2%) 59 56	41, 61, 99, 145	0
3	C	224/226 (99%)	-0.07	2 (0%) 81 80	39, 60, 101, 150	0
All	All	733/766 (95%)	0.26	37 (5%) 34 30	39, 76, 164, 205	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	187	GLU	5.8
1	A	171	VAL	3.9
1	A	77	CYS	3.6
1	A	216	LEU	3.6
1	A	84	VAL	3.5
1	A	143	TRP	3.4
1	A	82	CYS	3.4
1	A	73	ALA	3.3
1	A	70	PHE	3.1
1	A	142	GLY	3.0
1	A	166	CYS	2.8
1	A	78	LEU	2.7
1	A	164	VAL	2.7
3	C	26	GLY	2.6
1	A	177	MET	2.5
1	A	267	LEU	2.5
1	A	141	LEU	2.4
1	A	260	PRO	2.4
1	A	126	ALA	2.4
3	C	101	ASN	2.3
2	B	7	SER	2.3
1	A	64	ILE	2.3
2	B	1	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	76	GLY	2.2
1	A	252	ILE	2.2
1	A	162	GLY	2.2
1	A	258	PHE	2.2
1	A	138	THR	2.2
1	A	186	VAL	2.2
1	A	59	ALA	2.1
1	A	55	VAL	2.1
1	A	273	ALA	2.1
1	A	268	TRP	2.1
1	A	272	LEU	2.1
2	B	100	GLY	2.1
2	B	185	GLU	2.0
1	A	86	VAL	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](#)

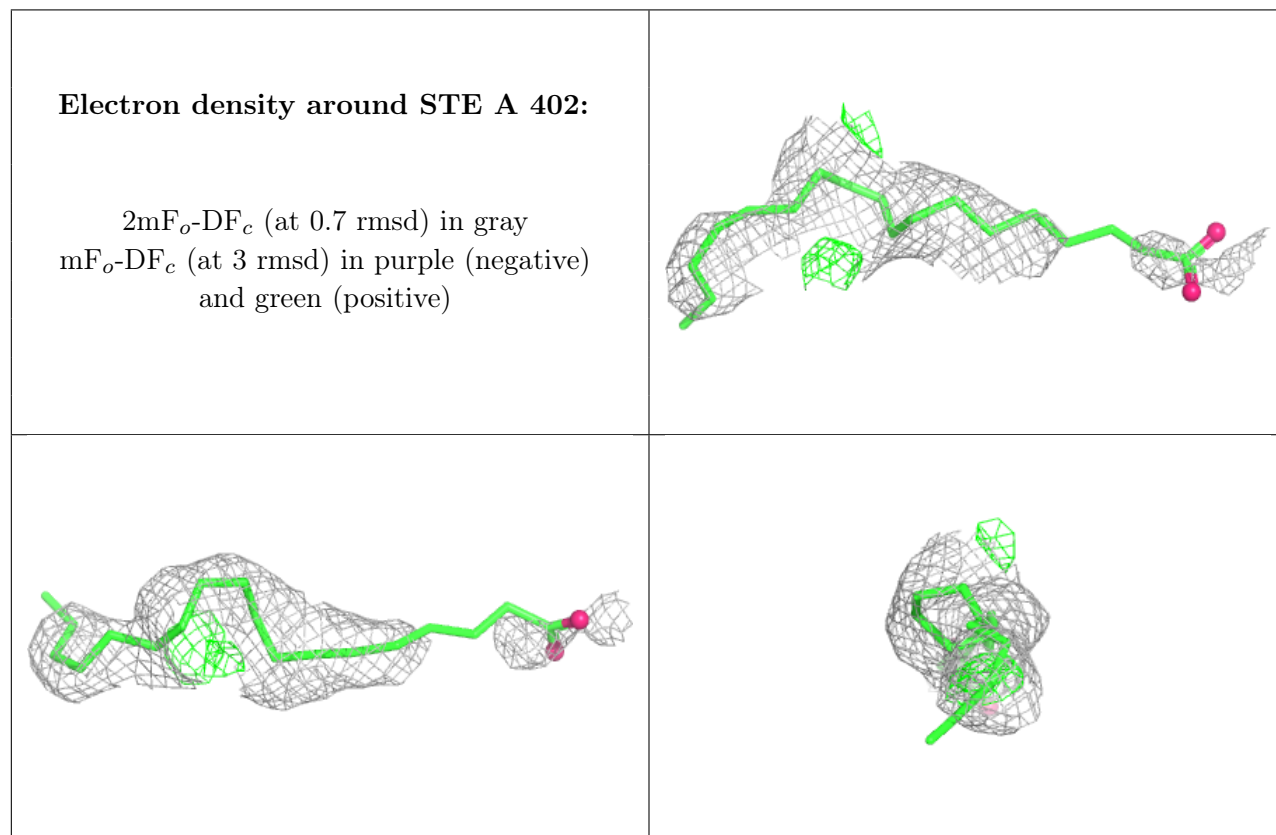
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

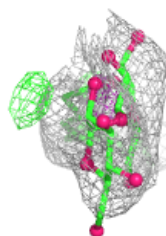
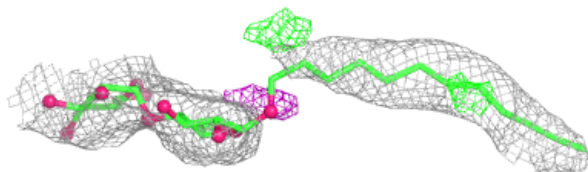
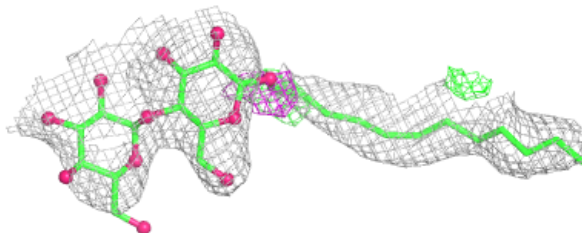
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	STE	A	402	20/20	0.64	0.18	113,126,140,142	0
6	LMT	A	408	35/35	0.68	0.14	92,139,157,158	0
5	STE	A	406	20/20	0.70	0.15	110,118,136,138	0
5	STE	A	405	20/20	0.76	0.19	101,116,139,140	0
5	STE	A	403	20/20	0.79	0.14	95,108,166,167	0
4	ZMA	A	401	25/25	0.82	0.18	149,163,194,198	0
5	STE	A	407	20/20	0.83	0.12	114,121,129,130	0
5	STE	A	404	20/20	0.84	0.14	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.

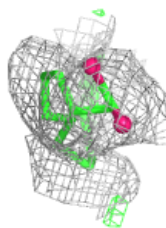
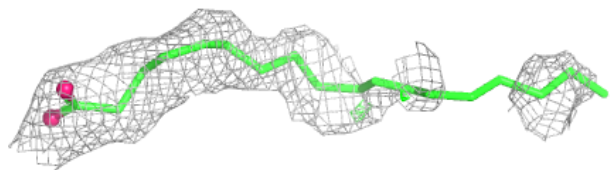
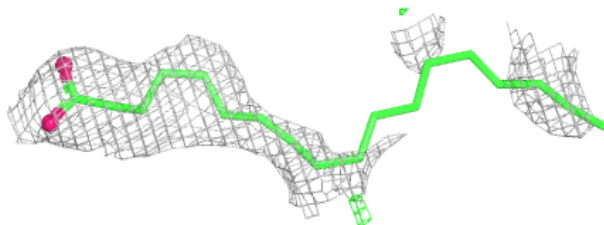


Electron density around LMT A 408:

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

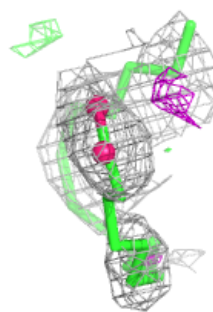
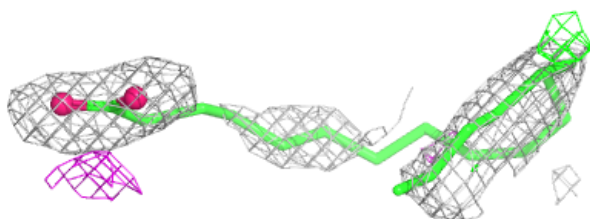
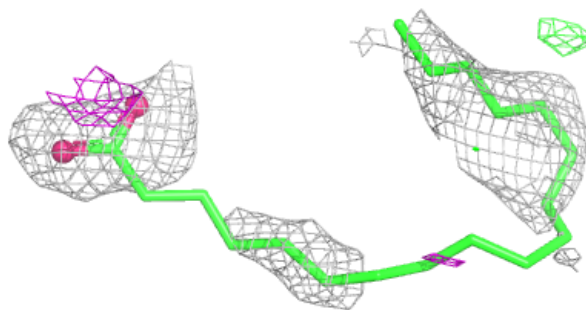
**Electron density around STE A 406:**

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

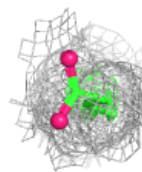
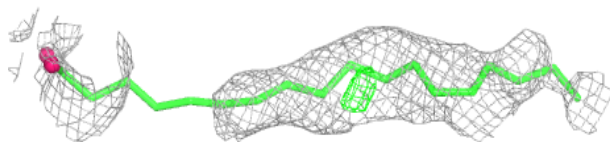
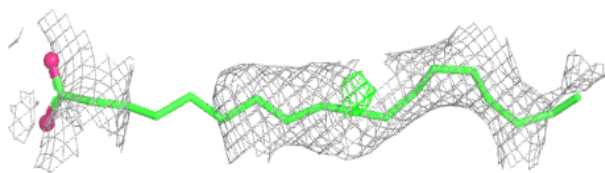


Electron density around STE A 405:

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

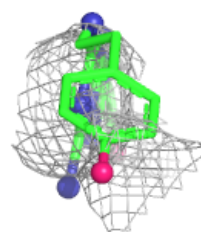
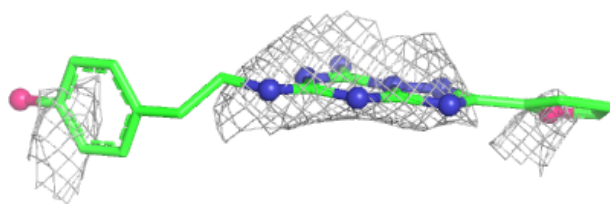
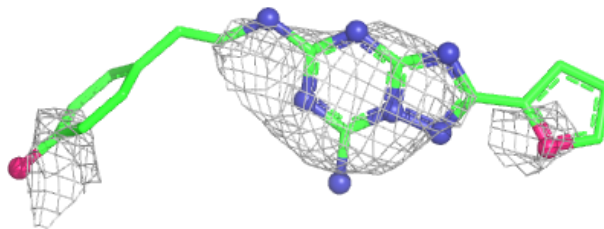
**Electron density around STE A 403:**

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

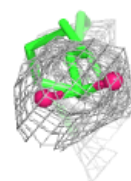
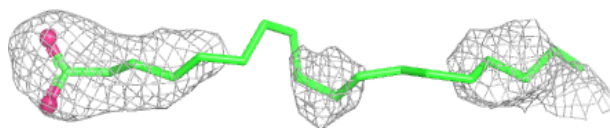
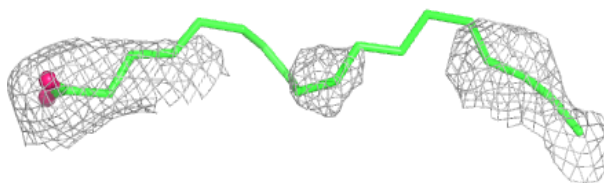


Electron density around ZMA A 401:

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

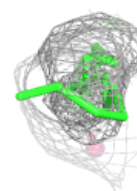
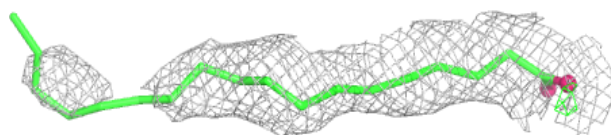
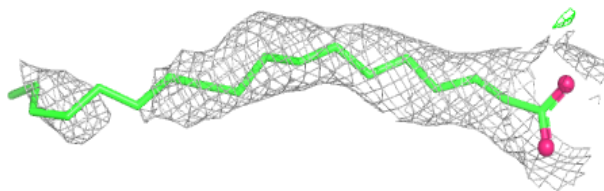
**Electron density around STE A 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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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.