



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:17 PM UTC

PDB ID : 5XLA / pdb_00005xla
Title : The structure of hemagglutinin G228S mutant from an avian-origin H4N6 influenza virus in complex with human receptor analog LSTc
Authors : Song, H.; Qi, J.; Gao, G.F.
Deposited on : 2017-05-10
Resolution : 2.10 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 ⓘ](#)) 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

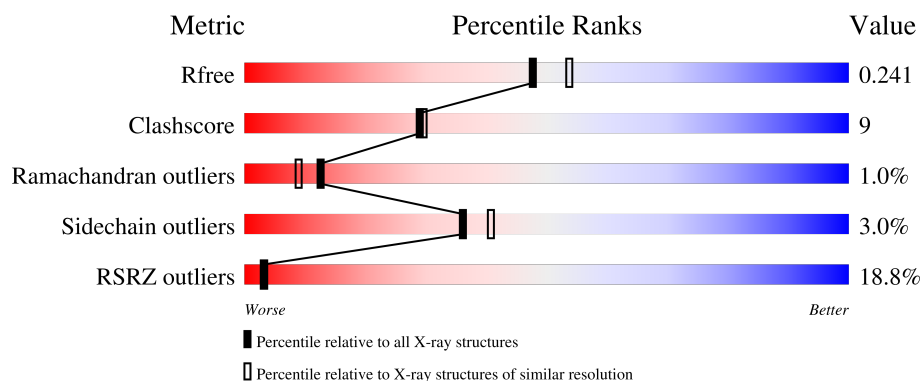
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	503	27% 76% 17% ...
1	B	503	10% 84% 12% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8332 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3861	2410	686	749	16			
1	B	490	Total	C	N	O	S	0	0	0
			3861	2410	686	749	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	SER	GLY	engineered mutation	UNP A3KF09
B	225	SER	GLY	engineered mutation	UNP A3KF09

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



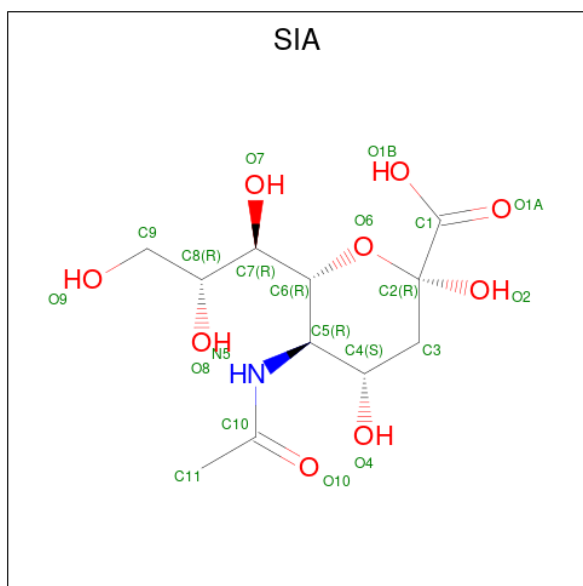
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		

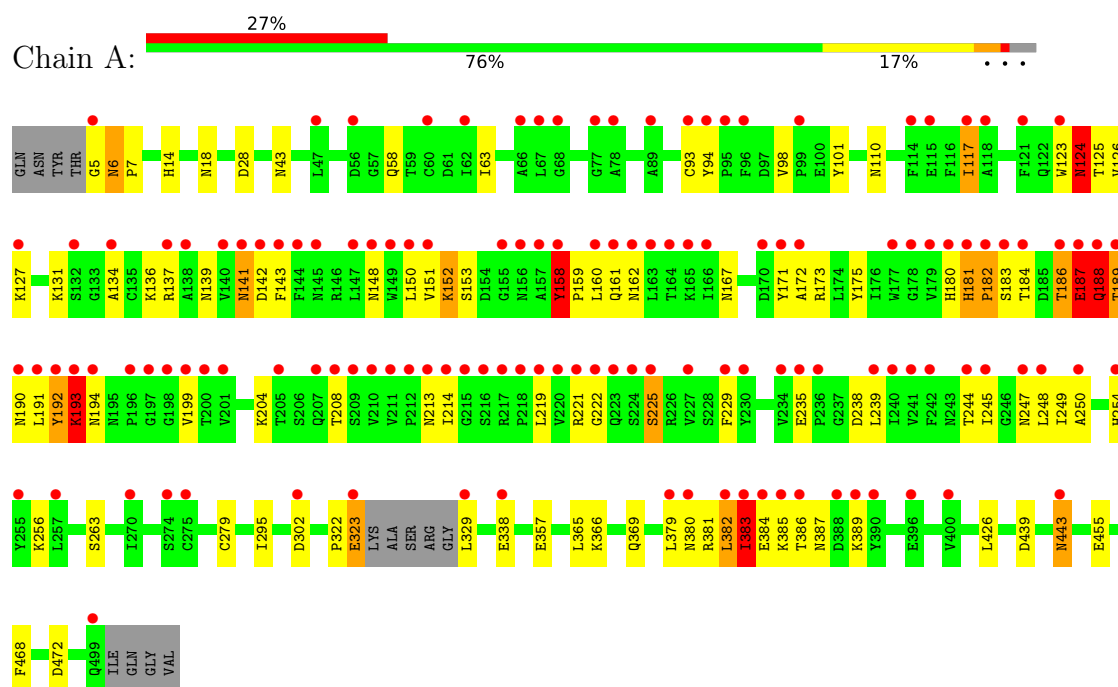
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		
4	B	322	Total	O	0	0
			322	322		

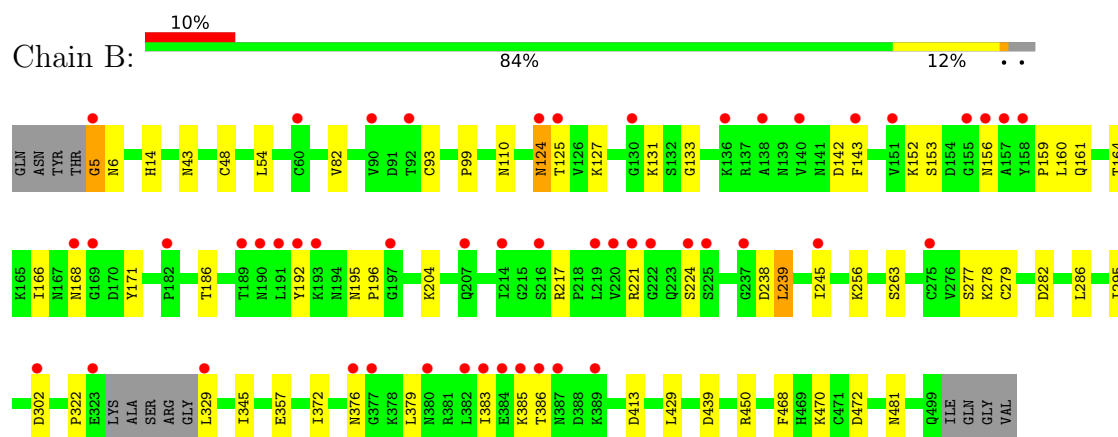
3 Residue-property plots [i](#)

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: Hemagglutinin



• Molecule 1: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.72Å 100.72Å 686.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.27 – 2.10 43.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.27-2.10) 94.1 (43.27-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.240 0.213 , 0.241	Depositor DCC
R_{free} test set	3991 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8332	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 48.49 % 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 8.5349e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SIA

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	0.47	1/3939 (0.0%)	0.92	10/5341 (0.2%)
1	B	0.36	0/3939	0.73	2/5341 (0.0%)
All	All	0.42	1/7878 (0.0%)	0.83	12/10682 (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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	LYS	CB-CG	-5.38	1.36	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	CA-C-N	-12.15	108.49	120.52
1	A	158	TYR	C-N-CA	-12.15	108.49	120.52
1	A	181	HIS	CA-C-N	9.59	131.82	119.84
1	A	181	HIS	C-N-CA	9.59	131.82	119.84
1	A	188	GLN	N-CA-C	-9.29	100.72	112.90
1	A	193	LYS	N-CA-C	8.66	129.25	110.80
1	A	189	THR	CA-C-N	-7.43	111.01	122.60
1	A	189	THR	C-N-CA	-7.43	111.01	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLN	CA-CB-CG	5.81	125.73	114.10
1	B	322	PRO	CA-C-N	5.16	131.00	121.70
1	B	322	PRO	C-N-CA	5.16	131.00	121.70
1	A	58	GLN	CB-CA-C	-5.09	110.72	116.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	GLU	Peptide
1	A	192	TYR	Peptide
1	B	5	GLY	Peptide

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	3861	0	3729	86	0
1	B	3861	0	3729	45	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0
3	A	21	0	18	0	0
3	B	21	0	18	1	0
4	A	218	0	0	9	0
4	B	322	0	0	13	0
All	All	8332	0	7520	133	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 9.

All (133) 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:B:385:LYS:HG2	1:B:386:THR:HG23	1.17	1.15
1:A:189:THR:HA	1:A:193:LYS:HA	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:NZ	4:A:701:HOH:O	1.93	1.02
1:B:5:GLY:N	4:B:701:HOH:O	1.94	1.00
1:B:5:GLY:HA2	1:B:468:PHE:HA	1.51	0.92
1:B:385:LYS:CG	1:B:386:THR:HG23	2.00	0.92
1:B:385:LYS:HG2	1:B:386:THR:CG2	2.03	0.87
1:A:184:THR:H	1:A:187:GLU:CG	1.90	0.83
1:A:443:ASN:OD1	4:A:702:HOH:O	1.97	0.82
1:A:443:ASN:C	1:A:443:ASN:HD22	1.90	0.79
1:A:338:GLU:OE1	4:A:703:HOH:O	2.02	0.78
1:A:188:GLN:HE22	1:A:192:TYR:HD2	1.33	0.76
1:A:204:LYS:HE2	1:A:238:ASP:HA	1.67	0.76
1:A:384:GLU:HG2	1:A:385:LYS:H	1.49	0.75
1:A:455:GLU:OE2	4:A:704:HOH:O	2.04	0.75
1:B:99:PRO:O	4:B:702:HOH:O	2.04	0.75
1:B:131:LYS:NZ	4:B:706:HOH:O	2.20	0.75
1:A:387:ASN:OD1	1:A:389:LYS:NZ	2.21	0.74
1:B:93:CYS:O	1:B:221:ARG:NH1	2.20	0.74
1:A:183:SER:H	1:A:187:GLU:HG3	1.52	0.74
1:A:151:VAL:HG23	1:A:191:LEU:HD12	1.69	0.73
1:A:184:THR:O	1:A:214:ILE:HG21	1.88	0.72
1:A:162:ASN:ND2	4:A:709:HOH:O	2.19	0.71
1:A:28:ASP:OD2	4:A:706:HOH:O	2.10	0.69
1:A:184:THR:H	1:A:187:GLU:HG2	1.56	0.69
1:A:189:THR:O	1:A:193:LYS:HG2	1.93	0.69
1:B:282:ASP:OD2	4:B:703:HOH:O	2.10	0.67
1:A:181:HIS:HB2	1:A:213:ASN:O	1.95	0.66
1:B:43:ASN:HB3	1:B:295:ILE:HD13	1.79	0.65
1:B:166:ILE:HG22	1:B:168:ASN:OD1	1.97	0.65
1:A:188:GLN:HE21	1:A:188:GLN:HA	1.61	0.64
1:A:322:PRO:O	1:A:323:GLU:HB2	1.98	0.64
1:A:369:GLN:OE1	4:A:708:HOH:O	2.14	0.64
1:A:188:GLN:NE2	1:A:192:TYR:HD2	1.95	0.64
1:A:188:GLN:HE21	1:A:188:GLN:CA	2.11	0.64
1:A:180:HIS:HB2	1:A:249:ILE:HD11	1.80	0.63
1:A:182:PRO:HB3	1:A:187:GLU:HB3	1.80	0.62
1:A:43:ASN:HB3	1:A:295:ILE:HD13	1.83	0.61
1:B:142:ASP:OD1	1:B:143:PHE:N	2.29	0.61
1:A:379:LEU:HD11	1:A:426:LEU:HD21	1.83	0.61
1:B:481:ASN:ND2	4:B:713:HOH:O	2.33	0.61
1:B:345:ILE:O	4:B:705:HOH:O	2.16	0.61
1:A:171:TYR:CE2	1:A:256:LYS:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:H	1:A:187:GLU:HG3	1.64	0.60
1:B:302:ASP:OD1	1:B:386:THR:HB	2.02	0.59
1:B:238:ASP:OD2	4:B:704:HOH:O	2.16	0.59
1:A:152:LYS:HD3	1:A:193:LYS:HZ2	1.67	0.58
1:A:159:PRO:O	1:A:161:GLN:NE2	2.37	0.57
1:B:357:GLU:HG3	4:B:940:HOH:O	2.05	0.57
1:A:142:ASP:CG	1:A:143:PHE:H	2.14	0.56
1:A:134:ALA:O	1:A:221:ARG:NH2	2.39	0.55
1:A:98:VAL:HG22	1:A:229:PHE:HB2	1.89	0.55
1:A:117:ILE:HD11	1:A:254:HIS:NE2	2.22	0.55
1:A:126:VAL:HG13	1:A:159:PRO:HD2	1.89	0.55
1:A:329:LEU:HG	1:A:439:ASP:OD1	2.07	0.55
1:B:450:ARG:NH2	4:B:716:HOH:O	2.39	0.55
1:A:182:PRO:CB	1:A:187:GLU:HB3	2.36	0.54
2:B:601:NAG:H83	4:B:800:HOH:O	2.06	0.54
1:B:171:TYR:CZ	1:B:256:LYS:HD2	2.42	0.54
1:A:5:GLY:HA2	1:A:468:PHE:HA	1.88	0.54
1:A:383:ILE:O	1:A:383:ILE:HG22	2.07	0.54
1:A:123:TRP:O	1:A:124:ASN:O	2.25	0.53
1:B:385:LYS:HG2	1:B:386:THR:N	2.24	0.53
1:A:18:ASN:ND2	4:A:705:HOH:O	2.04	0.52
1:A:127:LYS:HB3	1:A:151:VAL:CG1	2.39	0.52
1:B:329:LEU:HD21	4:B:772:HOH:O	2.08	0.52
1:A:152:LYS:NZ	1:A:190:ASN:HA	2.25	0.52
1:A:382:LEU:C	1:A:384:GLU:H	2.18	0.52
1:A:152:LYS:HD3	1:A:193:LYS:NZ	2.23	0.51
1:A:219:LEU:HG	1:A:222:GLY:HA2	1.92	0.50
1:A:443:ASN:O	1:A:443:ASN:ND2	2.38	0.50
1:A:125:THR:HG22	1:A:153:SER:OG	2.11	0.50
1:B:329:LEU:HG	1:B:439:ASP:OD1	2.11	0.50
1:B:125:THR:HG22	1:B:125:THR:O	2.12	0.50
1:A:175:TYR:CE2	1:A:254:HIS:HB3	2.46	0.50
1:B:217:ARG:HB2	1:B:224:SER:O	2.12	0.49
1:A:158:TYR:CD1	1:A:194:ASN:OD1	2.65	0.49
1:B:124:ASN:HB3	1:B:161:GLN:HE22	1.76	0.49
1:A:123:TRP:CD2	1:A:150:LEU:HD21	2.47	0.49
1:A:357:GLU:OE2	1:A:472:ASP:HB2	2.14	0.48
1:B:142:ASP:CG	1:B:143:PHE:H	2.20	0.48
1:A:6:ASN:HB3	1:A:7:PRO:HD3	1.96	0.47
1:B:127:LYS:HG3	1:B:153:SER:HA	1.97	0.47
1:A:158:TYR:CE1	1:A:194:ASN:OD1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ILE:HG23	1:B:376:ASN:ND2	2.30	0.47
1:A:383:ILE:O	1:A:383:ILE:CG2	2.62	0.46
1:A:63:ILE:HG13	1:A:101:TYR:CZ	2.51	0.46
1:A:386:THR:O	1:A:387:ASN:HB3	2.14	0.46
1:B:357:GLU:OE2	1:B:472:ASP:HB2	2.15	0.46
1:A:127:LYS:HB3	1:A:151:VAL:HG12	1.97	0.46
1:A:192:TYR:CZ	1:A:247:ASN:HA	2.50	0.46
2:A:601:NAG:H83	4:A:737:HOH:O	2.15	0.45
1:A:131:LYS:HD3	1:A:141:ASN:O	2.17	0.45
1:B:413:ASP:OD1	4:B:707:HOH:O	2.21	0.45
1:A:172:ALA:HB2	1:A:235:GLU:HG3	1.99	0.45
1:A:183:SER:N	1:A:187:GLU:HG3	2.25	0.45
1:A:188:GLN:HA	1:A:188:GLN:NE2	2.28	0.45
1:A:443:ASN:C	1:A:443:ASN:ND2	2.64	0.44
1:B:385:LYS:CD	1:B:386:THR:HG23	2.47	0.44
1:A:137:ARG:NE	1:A:142:ASP:OD2	2.24	0.44
1:A:142:ASP:OD1	1:A:143:PHE:N	2.48	0.44
1:A:93:CYS:SG	1:A:94:TYR:N	2.86	0.43
1:A:152:LYS:HE3	1:A:191:LEU:CA	2.47	0.43
1:A:171:TYR:CE2	1:A:173:ARG:HG2	2.53	0.43
1:B:54:LEU:HD22	1:B:82:VAL:HB	1.98	0.43
1:B:278:LYS:HB3	1:B:302:ASP:HB3	2.00	0.43
1:A:124:ASN:HB3	1:A:159:PRO:HG2	2.00	0.43
1:B:152:LYS:HD2	1:B:156:ASN:OD1	2.19	0.43
1:A:94:TYR:OH	1:A:225:SER:HB2	2.18	0.43
1:B:48:CYS:SG	1:B:277:SER:HB3	2.58	0.43
1:B:279:CYS:HB2	1:B:302:ASP:O	2.19	0.42
1:A:134:ALA:HB1	1:A:221:ARG:HB3	2.00	0.42
1:A:136:LYS:HD3	1:A:139:ASN:OD1	2.20	0.42
1:A:279:CYS:HB2	1:A:302:ASP:O	2.20	0.42
1:B:124:ASN:OD1	1:B:159:PRO:HG3	2.20	0.42
1:A:186:THR:HA	1:A:189:THR:HG22	2.02	0.42
1:B:133:GLY:N	3:B:602:SIA:O1B	2.53	0.42
1:A:136:LYS:HB3	1:A:139:ASN:HA	2.01	0.41
1:A:110:ASN:HA	1:A:263:SER:O	2.21	0.41
1:B:195:ASN:HA	1:B:196:PRO:HA	1.90	0.41
1:A:173:ARG:HD3	1:A:254:HIS:CE1	2.55	0.41
1:B:125:THR:HG22	1:B:153:SER:HB3	2.03	0.41
1:B:470:LYS:NZ	4:B:721:HOH:O	2.45	0.41
1:B:160:LEU:HD23	1:B:245:ILE:HG23	2.03	0.41
1:B:204:LYS:HE2	1:B:238:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:HB3	1:A:250:ALA:HB3	2.03	0.41
1:A:167:ASN:HA	1:A:173:ARG:CZ	2.51	0.40
1:B:164:THR:HG23	1:B:239:LEU:HD23	2.02	0.40
1:A:125:THR:HG22	1:A:125:THR:O	2.20	0.40
1:A:380:ASN:OD1	1:A:381:ARG:N	2.54	0.40
1:A:199:VAL:HG11	1:A:248:LEU:HD13	2.03	0.40
1:A:152:LYS:HZ1	1:A:190:ASN:HA	1.85	0.40
1:B:110:ASN:HA	1:B:263:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/503 (97%)	458 (94%)	21 (4%)	7 (1%)	9	5
1	B	486/503 (97%)	460 (95%)	23 (5%)	3 (1%)	21	18
All	All	972/1006 (97%)	918 (94%)	44 (4%)	10 (1%)	12	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	187	GLU
1	A	193	LYS
1	B	6	ASN
1	B	124	ASN
1	A	383	ILE
1	A	6	ASN
1	A	182	PRO
1	B	383	ILE
1	A	158	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/433 (98%)	405 (96%)	18 (4%)	26	27
1	B	423/433 (98%)	416 (98%)	7 (2%)	53	62
All	All	846/866 (98%)	821 (97%)	25 (3%)	36	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	117	ILE
1	A	124	ASN
1	A	141	ASN
1	A	152	LYS
1	A	160	LEU
1	A	186	THR
1	A	188	GLN
1	A	208	THR
1	A	225	SER
1	A	239	LEU
1	A	244	THR
1	A	245	ILE
1	A	323	GLU
1	A	365	LEU
1	A	382	LEU
1	A	383	ILE
1	A	443	ASN
1	B	14	HIS
1	B	186	THR
1	B	192	TYR
1	B	239	LEU
1	B	286	LEU
1	B	379	LEU
1	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	156	ASN
1	A	443	ASN
1	B	14	HIS
1	B	42	GLN
1	B	213	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	SIA	A	602	-	21,21,21	1.52	3 (14%)	24,31,31	1.25	1 (4%)
2	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
2	NAG	A	601	1	14,14,15	0.40	0	17,19,21	0.55	0
3	SIA	B	602	-	21,21,21	1.56	2 (9%)	24,31,31	1.66	1 (4%)

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	SIA	A	602	-	-	1/20/38/38	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	SIA	B	602	-	-	2/20/38/38	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	SIA	O6-C2	4.65	1.47	1.43
3	A	602	SIA	O6-C2	4.55	1.47	1.43
3	B	602	SIA	C2-C1	3.53	1.59	1.53
3	A	602	SIA	C2-C1	3.36	1.58	1.53
3	A	602	SIA	C7-C6	2.06	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	SIA	O1A-C1-C2	-6.55	112.92	123.85
3	A	602	SIA	O1A-C1-C2	-3.80	117.51	123.85
2	B	601	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

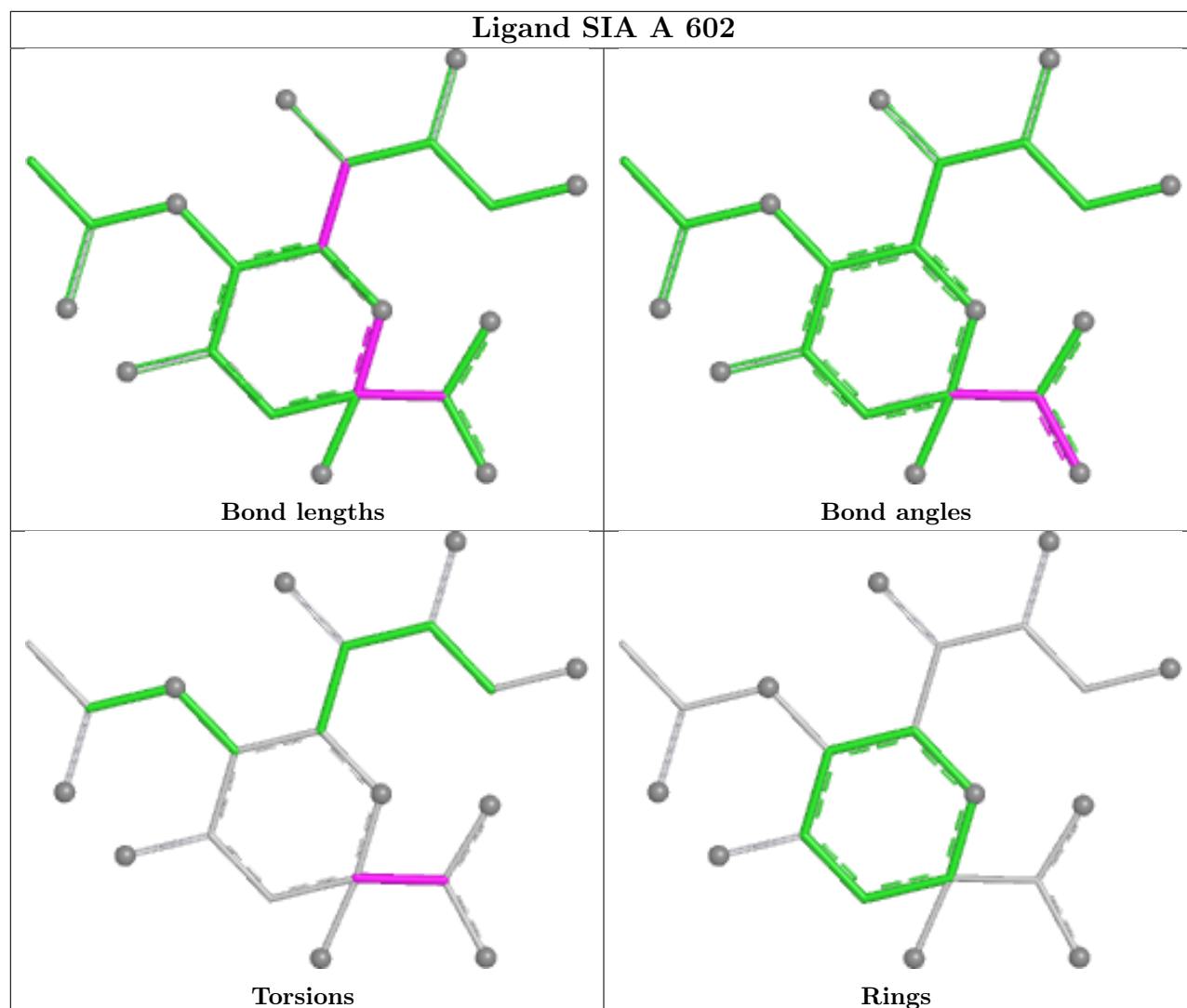
Mol	Chain	Res	Type	Atoms
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	B	601	NAG	C8-C7-N2-C2
2	B	601	NAG	O7-C7-N2-C2
3	A	602	SIA	O1A-C1-C2-O6
3	B	602	SIA	O1A-C1-C2-O6
3	B	602	SIA	O1B-C1-C2-O6

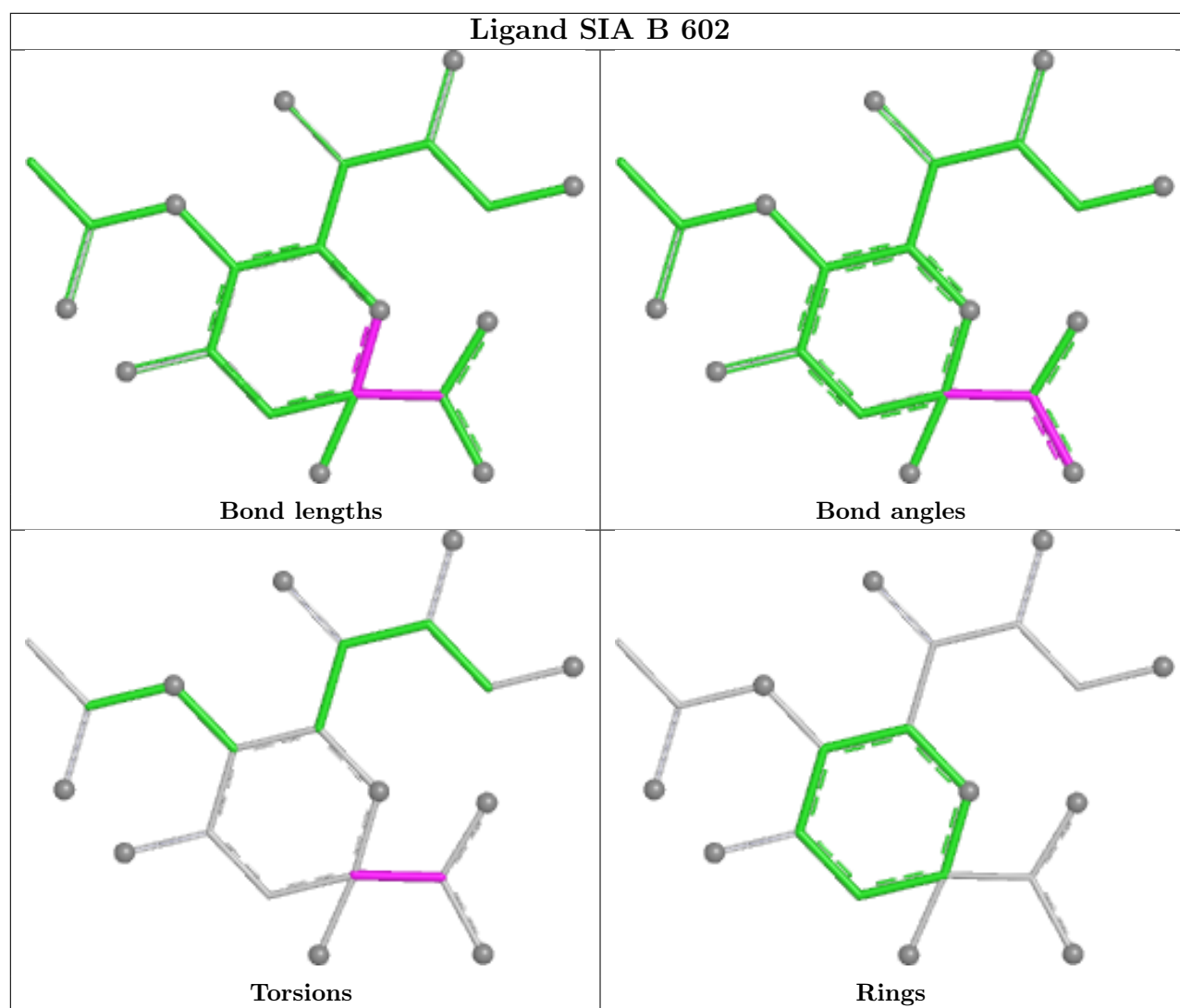
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAG	1	0
2	A	601	NAG	1	0
3	B	602	SIA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	490/503 (97%)	1.16	134 (27%) 1 1	19, 57, 130, 175	0
1	B	490/503 (97%)	0.44	50 (10%) 12 12	16, 36, 76, 138	0
All	All	980/1006 (97%)	0.80	184 (18%) 3 3	16, 43, 119, 175	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	8.9
1	B	5	GLY	7.5
1	A	163	LEU	6.6
1	A	222	GLY	6.3
1	A	158	TYR	6.3
1	A	386	THR	5.7
1	A	191	LEU	5.7
1	A	383	ILE	5.6
1	A	147	LEU	5.5
1	A	192	TYR	5.4
1	A	143	PHE	5.3
1	B	192	TYR	5.2
1	A	144	PHE	5.2
1	A	179	VAL	5.1
1	A	245	ILE	5.0
1	A	138	ALA	4.6
1	A	197	GLY	4.6
1	A	241	VAL	4.5
1	A	208	THR	4.5
1	A	157	ALA	4.5
1	A	117	ILE	4.4
1	A	181	HIS	4.3
1	B	221	ARG	4.3
1	A	123	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	157	ALA	4.2
1	B	125	THR	4.1
1	A	182	PRO	4.1
1	A	242	PHE	4.1
1	A	150	LEU	4.1
1	A	189	THR	4.1
1	A	156	ASN	4.0
1	A	170	ASP	4.0
1	B	386	THR	4.0
1	A	151	VAL	4.0
1	A	389	LYS	4.0
1	A	140	VAL	3.9
1	B	138	ALA	3.9
1	A	96	PHE	3.8
1	A	219	LEU	3.7
1	B	382	LEU	3.7
1	B	383	ILE	3.7
1	A	141	ASN	3.6
1	A	199	VAL	3.6
1	B	193	LYS	3.6
1	A	207	GLN	3.5
1	A	248	LEU	3.5
1	A	93	CYS	3.5
1	A	211	VAL	3.5
1	A	196	PRO	3.5
1	A	382	LEU	3.5
1	A	149	TRP	3.4
1	A	247	ASN	3.4
1	A	201	VAL	3.4
1	A	160	LEU	3.4
1	A	194	ASN	3.3
1	A	68	GLY	3.3
1	A	183	SER	3.3
1	A	121	PHE	3.3
1	B	380	ASN	3.3
1	B	140	VAL	3.3
1	A	134	ALA	3.3
1	A	214	ILE	3.3
1	A	239	LEU	3.3
1	A	210	VAL	3.2
1	B	124	ASN	3.2
1	A	164	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	178	GLY	3.2
1	B	245	ILE	3.2
1	A	216	SER	3.2
1	A	225	SER	3.2
1	B	60	CYS	3.2
1	A	250	ALA	3.1
1	A	221	ARG	3.1
1	A	67	LEU	3.1
1	B	219	LEU	3.1
1	B	214	ILE	3.1
1	A	132	SER	3.1
1	A	213	ASN	3.0
1	A	229	PHE	3.0
1	A	257	LEU	3.0
1	A	78	ALA	3.0
1	A	166	ILE	3.0
1	A	184	THR	3.0
1	A	94	TYR	3.0
1	A	47	LEU	3.0
1	A	218	PRO	3.0
1	A	172	ALA	2.9
1	A	240	ILE	2.9
1	B	158	TYR	2.9
1	B	151	VAL	2.9
1	B	329	LEU	2.8
1	A	200	THR	2.8
1	B	189	THR	2.8
1	B	191	LEU	2.8
1	A	187	GLU	2.8
1	A	148	ASN	2.8
1	A	275	CYS	2.8
1	A	235	GLU	2.7
1	A	171	TYR	2.7
1	A	186	THR	2.7
1	A	99	PRO	2.7
1	A	244	THR	2.7
1	A	388	ASP	2.7
1	B	222	GLY	2.7
1	A	145	ASN	2.7
1	A	56	ASP	2.7
1	A	127	LYS	2.7
1	A	66	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	193	LYS	2.6
1	A	215	GLY	2.6
1	A	236	PRO	2.6
1	A	198	GLY	2.6
1	A	379	LEU	2.6
1	A	212	PRO	2.6
1	A	390	TYR	2.5
1	B	302	ASP	2.5
1	A	142	ASP	2.5
1	A	188	GLN	2.5
1	B	207	GLN	2.5
1	B	384	GLU	2.5
1	A	254	HIS	2.5
1	A	385	LYS	2.5
1	A	223	GLN	2.5
1	A	95	PRO	2.5
1	B	182	PRO	2.5
1	A	329	LEU	2.5
1	A	234	VAL	2.4
1	A	115	GLU	2.4
1	A	161	GLN	2.4
1	B	385	LYS	2.4
1	A	155	GLY	2.4
1	A	60	CYS	2.4
1	B	225	SER	2.4
1	A	118	ALA	2.4
1	A	62	ILE	2.4
1	A	220	VAL	2.4
1	A	227	VAL	2.4
1	A	224	SER	2.4
1	B	136	LYS	2.4
1	A	162	ASN	2.3
1	A	302	ASP	2.3
1	A	270	ILE	2.3
1	B	216	SER	2.3
1	B	220	VAL	2.3
1	A	180	HIS	2.3
1	A	190	ASN	2.3
1	B	190	ASN	2.3
1	B	130	GLY	2.3
1	A	217	ARG	2.3
1	B	90	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	168	ASN	2.3
1	A	177	TRP	2.3
1	B	197	GLY	2.3
1	A	205	THR	2.3
1	A	77	GLY	2.3
1	A	443	ASN	2.2
1	B	376	ASN	2.2
1	A	384	GLU	2.2
1	A	396	GLU	2.2
1	B	143	PHE	2.2
1	B	237	GLY	2.2
1	A	89	ALA	2.2
1	B	323	GLU	2.2
1	B	92	THR	2.2
1	A	499	GLN	2.2
1	A	274	SER	2.2
1	A	323	GLU	2.1
1	A	209	SER	2.1
1	A	230	TYR	2.1
1	A	114	PHE	2.1
1	A	137	ARG	2.1
1	B	389	LYS	2.1
1	B	156	ASN	2.1
1	B	169	GLY	2.1
1	B	224	SER	2.1
1	A	380	ASN	2.1
1	A	165	LYS	2.1
1	A	400	VAL	2.1
1	B	155	GLY	2.0
1	B	377	GLY	2.0
1	A	338	GLU	2.0
1	B	387	ASN	2.0
1	B	275	CYS	2.0
1	A	255	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

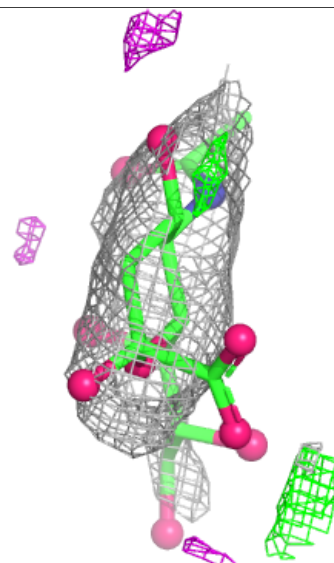
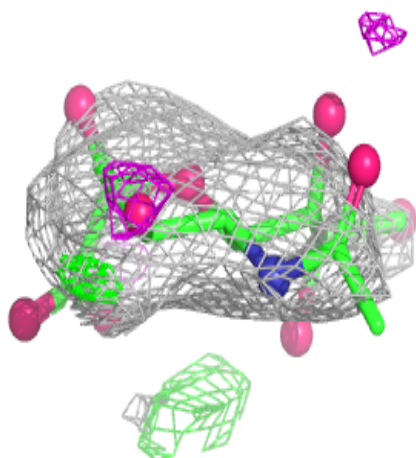
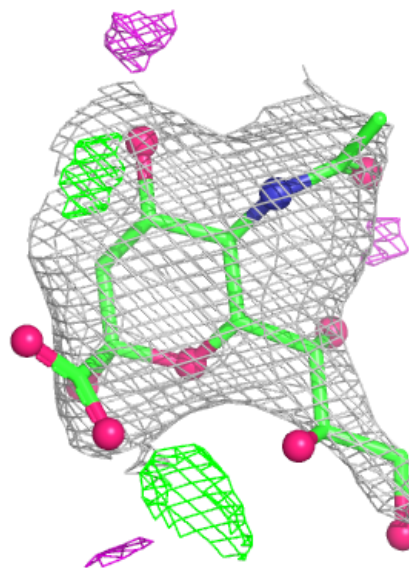
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SIA	A	602	21/21	0.58	0.19	113,123,128,129	0
3	SIA	B	602	21/21	0.80	0.13	65,72,78,79	0
2	NAG	A	601	14/15	0.86	0.11	42,48,53,64	0
2	NAG	B	601	14/15	0.87	0.09	28,32,36,46	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.

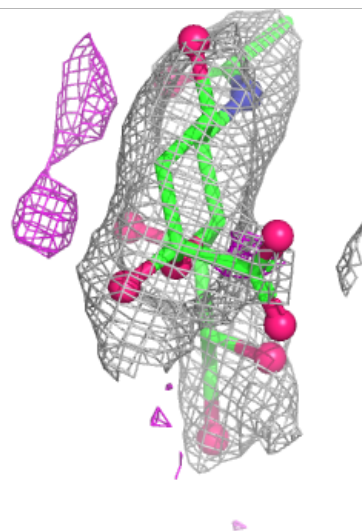
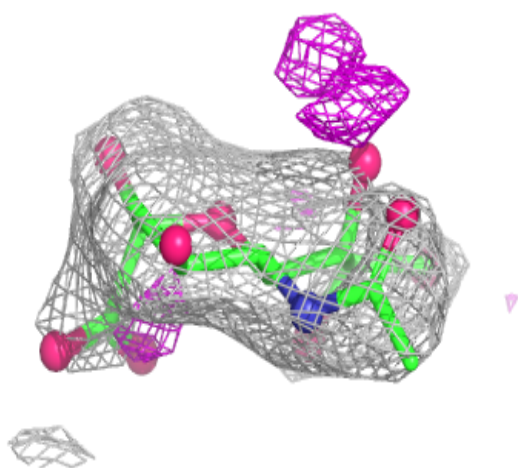
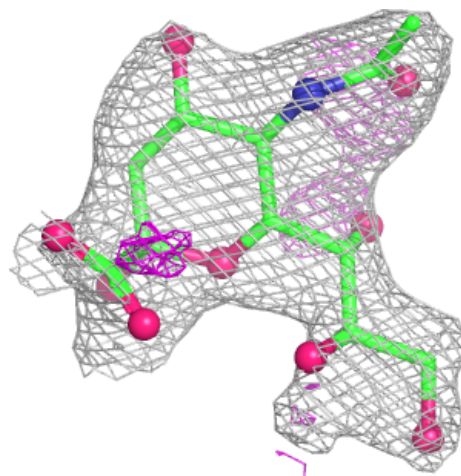
Electron density around SIA A 602:

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



Electron density around SIA B 602:

$2mF_o-DF_c$ (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.