



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:43 AM UTC

PDB ID : 2WU3 / pdb_00002wu3
Title : CRYSTAL STRUCTURE OF MOUSE ACETYLCHOLINESTERASE IN
COMPLEX WITH FENAMIPHOS AND HI-6
Authors : Hornberg, A.; Artursson, E.; Warme, R.; Pang, Y.-P.; Ekstrom, F.
Deposited on : 2009-09-28
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 ⓘ](#)) 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

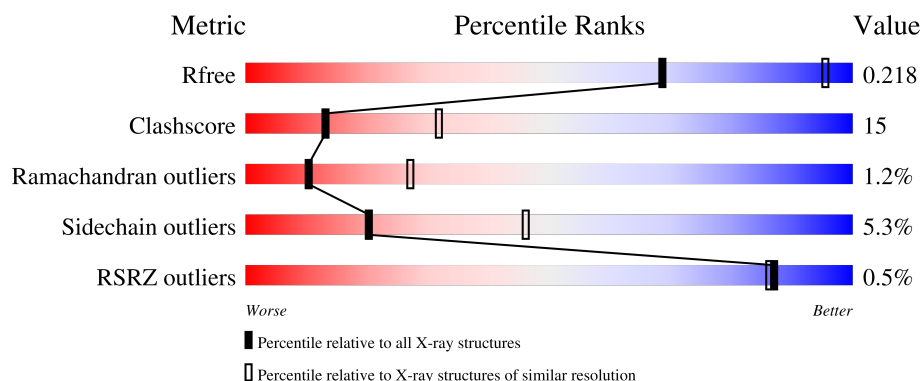
1 Overall quality at a glance

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	548	 72% 24% . .
1	B	548	 % 67% 26% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HI6	A	601	-	-	X	-
2	HI6	B	601	-	-	X	-
3	NAG	A	603	X	-	-	-
4	P6G	A	604	-	X	-	-

2 Entry composition [i](#)

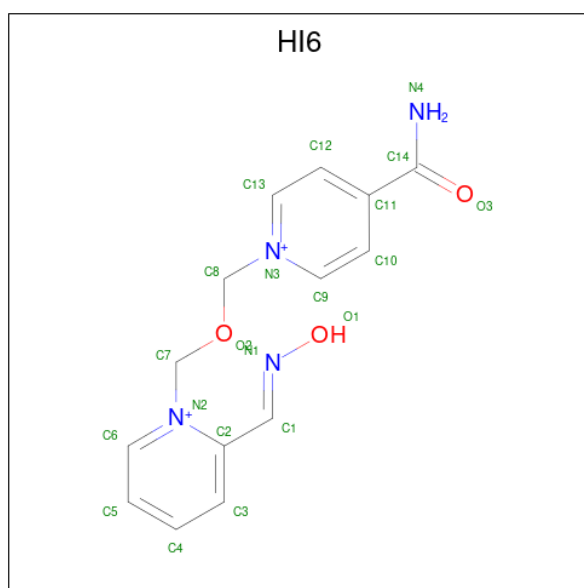
There are 6 unique types of molecules in this entry. The entry contains 8805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

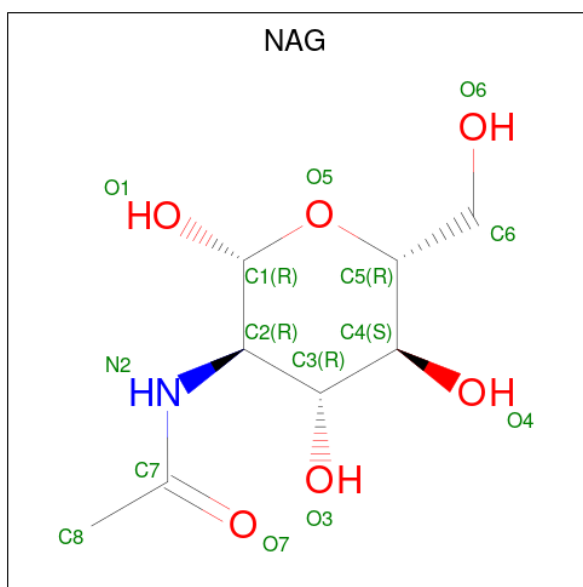
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	P	S	0	2	0
			4239	2715	733	775	2	14			
1	B	533	Total	C	N	O	P	S	0	1	0
			4184	2684	724	760	2	14			

- Molecule 2 is 4-(AMINOCARBONYL)-1-[(2-[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL}METHOXY)METHYL]PYRIDINIUM (CCD ID: HI6) (formula: C₁₄H₁₆N₄O₃).



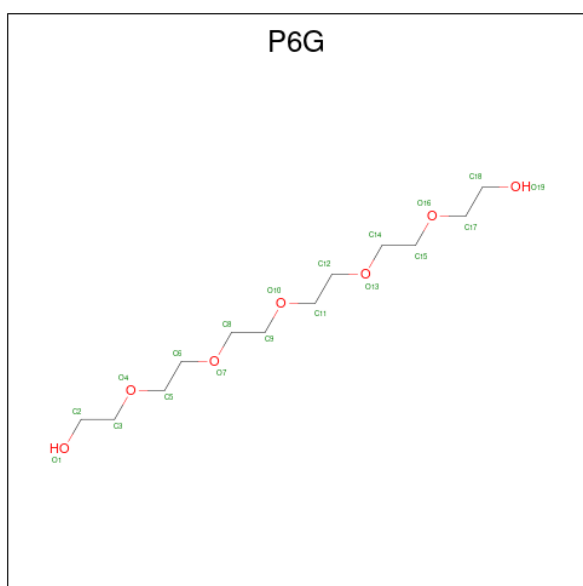
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



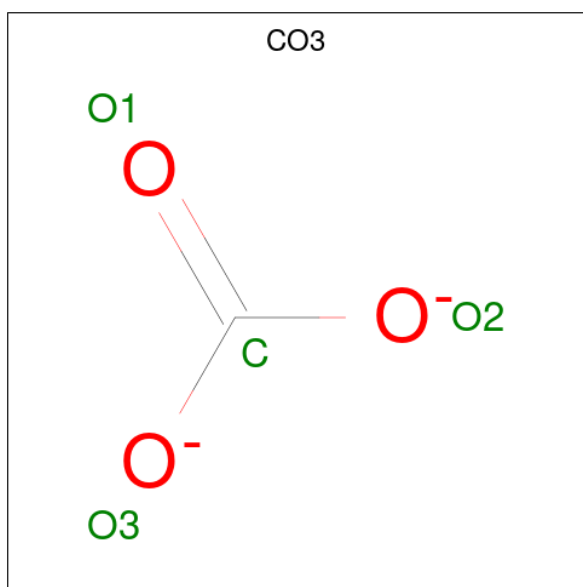
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	B	1	Total	C	O	0	0
			4	1	3		

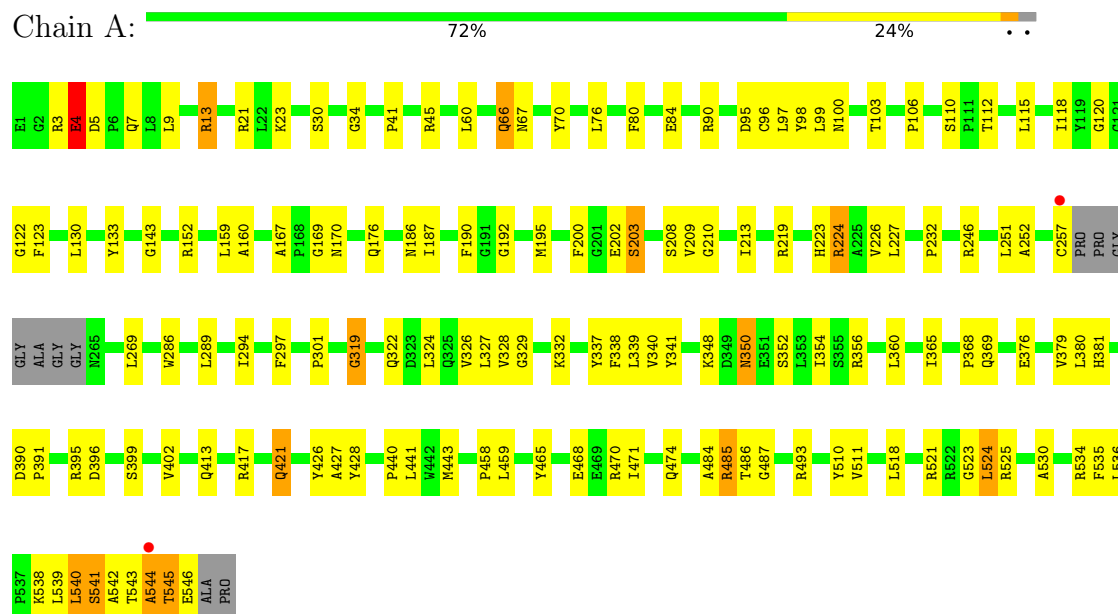
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	B	126	Total	O	0	0
			126	126		

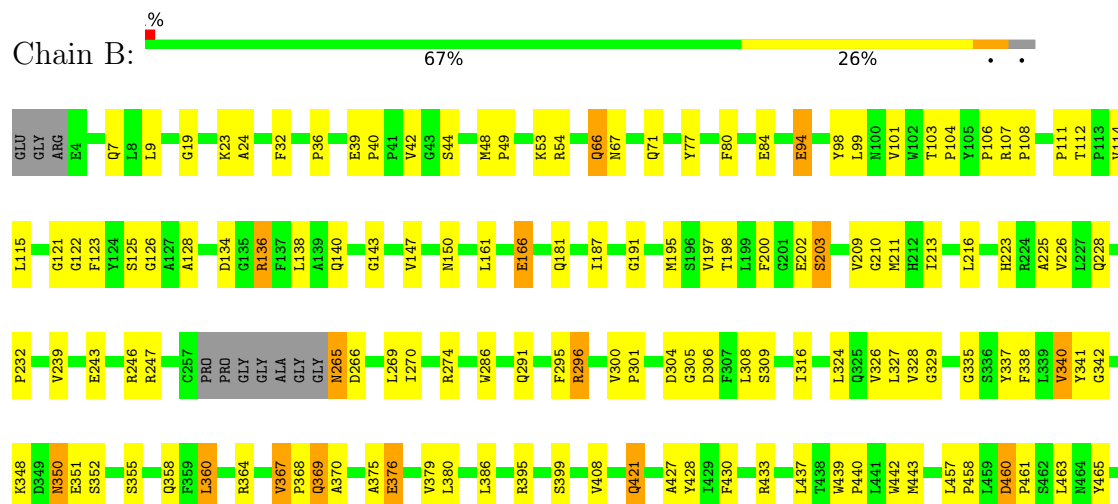
3 Residue-property plots [i](#)

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: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.76Å 111.23Å 227.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.02 – 2.70 29.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.02-2.70) 99.9 (29.02-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.171 , 0.226 0.166 , 0.218	Depositor DCC
R_{free} test set	1098 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.2	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	0.96	EDS
Total number of atoms	8805	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SXE, NAG, P6G, HI6, CO3

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	0.66	0/4334	1.00	11/5919 (0.2%)
1	B	0.62	0/4276	0.97	8/5842 (0.1%)
All	All	0.64	0/8610	0.99	19/11761 (0.2%)

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	541	SER	N-CA-C	-6.97	95.95	110.80
1	B	491	ASP	CA-C-N	6.25	126.37	119.87
1	B	491	ASP	C-N-CA	6.25	126.37	119.87
1	A	390	ASP	CA-C-N	5.93	126.08	119.32
1	A	390	ASP	C-N-CA	5.93	126.08	119.32
1	A	289	LEU	CA-C-N	5.89	125.27	118.85
1	A	289	LEU	C-N-CA	5.89	125.27	118.85
1	B	460	ASP	CA-C-N	5.79	125.16	118.85
1	B	460	ASP	C-N-CA	5.79	125.16	118.85
1	B	266	ASP	N-CA-C	5.78	117.27	110.97
1	A	209	VAL	N-CA-C	-5.67	104.84	110.62
1	B	367	VAL	CA-C-N	5.67	125.34	119.56
1	B	367	VAL	C-N-CA	5.67	125.34	119.56
1	A	167	ALA	CA-C-N	5.58	125.20	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ALA	C-N-CA	5.58	125.20	119.56
1	A	96	CYS	N-CA-CB	-5.25	101.61	110.49
1	A	485	ARG	N-CA-C	5.13	116.87	111.28
1	A	90	ARG	N-CA-C	-5.06	101.60	109.14
1	B	408	VAL	N-CA-C	5.01	115.62	110.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	540	LEU	Peptide
1	A	95	ASP	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	4239	0	4131	118	0
1	B	4184	0	4080	135	0
2	A	18	0	14	11	0
2	B	18	0	14	9	0
3	A	28	0	26	1	0
4	A	19	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	165	0	0	3	0
6	B	126	0	0	4	0
All	All	8805	0	8289	250	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 15.

All (250) 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:350:ASN:HD22	1:A:352:SER:H	1.09	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLN:HE22	1:B:107:ARG:H	0.96	0.95
1:A:350:ASN:ND2	1:A:352:SER:H	1.67	0.91
1:B:7:GLN:NE2	1:B:107:ARG:H	1.71	0.88
1:A:350:ASN:OD1	3:A:602:NAG:C1	2.22	0.87
1:B:286:TRP:CH2	2:B:601:HI6:H81	2.12	0.84
1:B:350:ASN:HD22	1:B:352:SER:H	1.23	0.83
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.60	0.82
1:B:355:SER:H	1:B:358:GLN:HE21	1.23	0.82
1:A:210:GLY:HA3	1:A:232:PRO:HG3	1.63	0.80
1:B:66:GLN:HE21	1:B:67:ASN:H	1.30	0.79
1:B:497:SER:HB3	1:B:498:PRO:O	1.82	0.79
1:A:176:GLN:HE22	1:A:208:SER:HB3	1.46	0.79
1:B:350:ASN:ND2	1:B:352:SER:H	1.82	0.78
1:A:381:HIS:HA	4:A:604:P6G:H31	1.69	0.75
1:A:417:ARG:HH21	1:A:421:GLN:HE22	1.31	0.74
1:A:286:TRP:CZ2	2:A:601:HI6:H82	2.23	0.74
1:A:224:ARG:HG3	1:A:224:ARG:HH11	1.53	0.74
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.70	0.73
1:A:286:TRP:CH2	2:A:601:HI6:H82	2.24	0.72
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.70	0.72
1:A:542:ALA:HB2	6:A:2110:HOH:O	1.89	0.72
1:A:224:ARG:HG3	1:A:224:ARG:NH1	2.05	0.71
1:A:341:TYR:CD1	2:A:601:HI6:H72	2.24	0.71
1:B:48:MET:HE3	1:B:166:GLU:HA	1.74	0.69
1:B:112:THR:HG21	1:B:143:GLY:O	1.92	0.68
1:A:350:ASN:HD22	1:A:352:SER:N	1.88	0.68
1:A:7:GLN:O	1:A:7:GLN:HG3	1.94	0.67
1:B:243:GLU:O	1:B:247:ARG:HG3	1.95	0.67
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.75	0.67
1:A:66:GLN:HE21	1:A:67:ASN:H	1.44	0.66
1:B:202:GLU:O	1:B:203[A]:SXE:HBC1	1.96	0.66
1:B:509:GLN:HG3	6:B:756:HOH:O	1.96	0.66
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.31	0.66
1:A:203[B]:SXE:H2C2	2:A:601:HI6:H4	1.77	0.65
1:B:71:GLN:HA	6:B:766:HOH:O	1.96	0.65
1:A:485:ARG:HB3	1:A:486:THR:HG23	1.78	0.65
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.77	0.65
1:A:350:ASN:HD22	1:A:350:ASN:C	2.05	0.64
1:B:540:LEU:C	1:B:542:ALA:H	2.07	0.62
1:A:203[A]:SXE:C5	2:A:601:HI6:H4	2.29	0.62
1:A:459:LEU:HD23	1:A:470:ARG:HG3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PRO:HG2	1:B:369:GLN:HG3	1.82	0.62
1:A:319:GLY:O	1:A:421:GLN:HG2	2.01	0.61
1:A:341:TYR:CE1	2:A:601:HI6:H72	2.35	0.61
1:A:224:ARG:HH11	1:A:224:ARG:CG	2.13	0.61
1:A:376:GLU:OE1	1:B:538:LYS:HD3	2.00	0.61
1:A:380:LEU:HD22	1:B:535:PHE:HB2	1.83	0.61
1:B:7:GLN:HE22	1:B:107:ARG:N	1.81	0.60
1:B:337:TYR:HE2	2:B:601:HI6:C4	2.15	0.60
1:A:337:TYR:HA	1:A:443:MET:HE2	1.84	0.60
1:A:203[B]:SXE:C2	2:A:601:HI6:H4	2.31	0.60
1:B:71:GLN:HE22	1:B:126:GLY:H	1.50	0.59
1:B:497:SER:CB	1:B:498:PRO:O	2.51	0.59
1:A:545:THR:O	1:A:546:GLU:HB3	2.02	0.59
1:B:122:GLY:O	1:B:123:PHE:HB2	2.02	0.59
1:A:380:LEU:HB3	4:A:604:P6G:H51	1.85	0.58
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.85	0.58
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.39	0.57
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.85	0.57
1:B:42:VAL:HG12	1:B:94:GLU:HB3	1.86	0.57
1:B:337:TYR:HE2	2:B:601:HI6:H4	1.69	0.57
1:A:470:ARG:O	1:A:474:GLN:HG3	2.03	0.57
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.05	0.56
1:B:514:ASN:C	1:B:514:ASN:HD22	2.13	0.56
1:B:367:VAL:HG12	1:B:370:ALA:HB2	1.87	0.56
1:B:470:ARG:O	1:B:474:GLN:HG3	2.05	0.56
1:A:13:ARG:NH2	6:A:2001:HOH:O	2.38	0.56
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.40	0.56
1:A:203[B]:SXE:H3C1	1:A:297:PHE:CZ	2.40	0.56
1:A:539:LEU:O	1:A:540:LEU:HD23	2.05	0.55
1:A:213:ILE:O	1:A:219:ARG:HD3	2.05	0.55
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.42	0.55
1:B:328:VAL:O	1:B:427:ALA:HA	2.07	0.55
1:A:545:THR:HG22	1:A:546:GLU:H	1.71	0.55
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.41	0.55
1:B:128:ALA:H	1:B:150:ASN:HD21	1.55	0.55
1:A:545:THR:HG22	1:A:546:GLU:N	2.22	0.54
1:B:66:GLN:HE21	1:B:67:ASN:N	2.02	0.54
1:B:430:PHE:HE2	1:B:476:LEU:HD11	1.72	0.54
1:A:210:GLY:CA	1:A:232:PRO:HG3	2.37	0.54
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.87	0.54
1:B:210:GLY:CA	1:B:232:PRO:HG3	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:HB	1:B:301:PRO:HD2	1.90	0.53
1:A:202:GLU:O	1:A:203[A]:SXE:HBC1	2.09	0.53
1:A:350:ASN:ND2	1:A:352:SER:N	2.46	0.53
1:A:511:VAL:HG11	1:A:518:LEU:HD13	1.91	0.53
1:B:265:ASN:C	1:B:265:ASN:OD1	2.52	0.53
1:A:76:LEU:HD22	1:A:341:TYR:CD1	2.44	0.53
1:B:211:MET:HE3	1:B:232:PRO:HA	1.90	0.53
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.91	0.52
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.91	0.52
1:A:350:ASN:ND2	1:A:350:ASN:C	2.67	0.52
1:A:545:THR:O	1:A:546:GLU:CB	2.58	0.52
1:A:203[B]:SXE:H3C1	1:A:297:PHE:HZ	1.73	0.52
1:A:459:LEU:CD2	1:A:470:ARG:HG3	2.40	0.51
1:B:80:PHE:O	1:B:84:GLU:HB2	2.09	0.51
1:A:380:LEU:HB3	4:A:604:P6G:C5	2.40	0.51
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.40	0.51
1:B:493:ARG:O	1:B:494:ASP:CB	2.59	0.51
1:A:203[A]:SXE:H5C1	2:A:601:HI6:C4	2.41	0.51
1:B:108:PRO:HG2	1:B:191:GLY:HA3	1.92	0.51
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.40	0.51
1:B:202:GLU:O	1:B:203[B]:SXE:HBC1	2.04	0.51
1:B:497:SER:CB	1:B:498:PRO:C	2.84	0.51
1:A:41:PRO:HG2	1:A:152:ARG:HD3	1.93	0.51
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.46	0.51
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.11	0.51
1:B:115:LEU:HD23	1:B:198:THR:HB	1.93	0.50
1:A:339:LEU:HD11	1:A:399:SER:HA	1.93	0.50
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.93	0.50
1:B:337:TYR:CE2	2:B:601:HI6:H4	2.46	0.50
1:B:36:PRO:HB2	1:B:53:LYS:HD3	1.93	0.50
1:B:495:SER:O	1:B:496:LYS:O	2.30	0.50
1:B:286:TRP:CZ2	2:B:601:HI6:H81	2.47	0.49
1:A:543:THR:O	1:A:543:THR:HG23	2.12	0.49
1:B:228:GLN:HE21	1:B:480:TRP:HE1	1.61	0.49
1:A:224:ARG:HD3	1:A:487:GLY:HA2	1.94	0.49
1:B:71:GLN:NE2	1:B:126:GLY:H	2.11	0.49
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.47	0.49
1:A:252:ALA:HB1	1:A:257:CYS:HB2	1.93	0.49
1:A:471:ILE:HA	1:A:474:GLN:HE21	1.77	0.49
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.47	0.49
1:B:440:PRO:HG2	1:B:443:MET:HG3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:C	1:A:203[A]:SXE:H2C2	2.37	0.49
1:B:350:ASN:HD22	1:B:351:GLU:N	2.11	0.49
1:A:328:VAL:O	1:A:427:ALA:HA	2.13	0.49
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.48	0.49
1:B:296:ARG:NH1	1:B:369:GLN:HE21	2.11	0.48
1:A:365:ILE:O	1:A:368:PRO:HD3	2.14	0.48
1:A:4:GLU:HG2	1:A:9:LEU:HD21	1.96	0.48
1:B:376:GLU:O	1:B:380:LEU:HG	2.13	0.48
1:A:66:GLN:HE21	1:A:67:ASN:N	2.09	0.48
1:B:7:GLN:NE2	1:B:107:ARG:N	2.52	0.48
1:A:34:GLY:H	1:A:100:ASN:ND2	2.12	0.48
1:A:60:LEU:C	1:A:60:LEU:HD23	2.38	0.48
1:B:352:SER:O	1:B:395:ARG:HG3	2.13	0.48
1:B:48:MET:CE	1:B:166:GLU:HA	2.43	0.47
1:B:71:GLN:NE2	1:B:125:SER:HB2	2.29	0.47
1:A:348:LYS:O	1:A:440:PRO:HG3	2.15	0.47
1:A:203[B]:SXE:H1	1:A:203[B]:SXE:H4C2	1.61	0.47
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.96	0.47
1:B:355:SER:OG	1:B:358:GLN:HG3	2.15	0.47
1:B:296:ARG:HH12	1:B:369:GLN:NE2	2.13	0.47
1:B:360:LEU:N	1:B:360:LEU:HD23	2.30	0.47
1:B:115:LEU:HD21	1:B:484:ALA:HB2	1.96	0.47
1:A:13:ARG:H	1:A:186:ASN:ND2	2.13	0.46
1:A:354:ILE:O	1:A:391:PRO:HA	2.15	0.46
1:B:99:LEU:C	1:B:99:LEU:HD12	2.41	0.46
1:B:269:LEU:C	1:B:269:LEU:HD23	2.40	0.46
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.45	0.46
1:A:187:ILE:HG13	1:A:192:GLY:HA3	1.96	0.46
1:A:525:ARG:HD3	6:A:2138:HOH:O	2.16	0.46
1:A:122:GLY:O	1:A:123:PHE:HB2	2.15	0.46
1:A:468:GLU:CD	1:A:468:GLU:H	2.24	0.46
1:A:159:LEU:C	1:A:159:LEU:HD23	2.41	0.46
1:A:523:GLY:HA3	1:B:386:LEU:HD21	1.97	0.45
1:A:543:THR:O	1:A:544:ALA:HB2	2.16	0.45
1:A:80:PHE:O	1:A:84:GLU:HG2	2.16	0.45
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.99	0.45
1:A:530:ALA:O	1:A:534:ARG:HB2	2.15	0.45
1:B:7:GLN:NE2	1:B:106:PRO:HA	2.32	0.45
1:B:48:MET:HB3	1:B:49:PRO:HD2	1.98	0.45
1:B:107:ARG:HE	1:B:107:ARG:HB2	1.59	0.45
1:B:128:ALA:H	1:B:150:ASN:ND2	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:HA	1:B:191:GLY:O	2.17	0.45
1:A:360:LEU:HD22	1:A:379:VAL:HG21	1.99	0.45
1:B:364:ARG:O	1:B:368:PRO:HA	2.17	0.45
1:B:540:LEU:C	1:B:542:ALA:N	2.73	0.45
1:B:340:VAL:HG11	1:B:443:MET:CE	2.46	0.45
1:B:305:GLY:HA2	1:B:309:SER:HA	1.99	0.45
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.76	0.45
1:B:265:ASN:ND2	6:B:703:HOH:O	2.50	0.44
1:A:203[A]:SXE:H5C3	2:A:601:HI6:H4	1.97	0.44
1:B:19:GLY:HA3	1:B:32:PHE:CD2	2.53	0.44
1:A:103:THR:HG21	1:A:190:PHE:HB3	2.00	0.44
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.00	0.44
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.17	0.44
1:A:341:TYR:CD1	2:A:601:HI6:C7	2.98	0.44
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.53	0.44
1:B:228:GLN:NE2	1:B:480:TRP:HE1	2.15	0.44
1:A:356:ARG:O	1:A:360:LEU:HG	2.17	0.43
1:B:138:LEU:HA	1:B:477:MET:HE3	1.99	0.43
1:A:5:ASP:C	1:A:5:ASP:OD1	2.59	0.43
1:A:41:PRO:HG3	1:A:97:LEU:CD1	2.48	0.43
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.00	0.43
1:B:341:TYR:CD2	2:B:601:HI6:H72	2.53	0.43
1:A:30:SER:HB2	1:A:103:THR:OG1	2.18	0.43
1:A:535:PHE:CE2	4:A:604:P6G:H91	2.53	0.43
1:B:481:THR:OG1	1:B:485:ARG:NH2	2.51	0.43
1:A:7:GLN:CD	1:A:106:PRO:HB3	2.44	0.43
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.54	0.43
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.48	0.43
1:B:497:SER:H	1:B:498:PRO:HA	1.82	0.43
1:B:39:GLU:HA	1:B:40:PRO:HD3	1.91	0.43
1:B:300:VAL:HB	1:B:301:PRO:CD	2.48	0.43
1:A:112:THR:HG21	1:A:143:GLY:O	2.19	0.43
1:A:200:PHE:CB	1:A:226:VAL:HB	2.49	0.42
1:A:66:GLN:HE21	1:A:66:GLN:CA	2.31	0.42
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.18	0.42
1:B:461:PRO:C	1:B:463:LEU:H	2.27	0.42
1:B:536:LEU:HB3	1:B:537:PRO:HD3	2.01	0.42
1:B:66:GLN:NE2	1:B:67:ASN:H	2.08	0.42
1:B:460:ASP:O	1:B:463:LEU:HB2	2.20	0.42
1:B:497:SER:HB2	1:B:498:PRO:C	2.45	0.42
1:A:269:LEU:C	1:A:269:LEU:HD23	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG12	1:A:328:VAL:HG13	2.02	0.42
1:B:209:VAL:O	1:B:213:ILE:HG13	2.20	0.42
1:A:538:LYS:C	1:A:540:LEU:H	2.27	0.42
1:A:327:LEU:HD12	1:A:426:TYR:O	2.20	0.42
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.55	0.42
1:A:195:MET:C	1:A:223:HIS:CE1	2.98	0.41
1:B:286:TRP:CH2	2:B:601:HI6:C8	2.95	0.41
1:B:457:LEU:N	1:B:458:PRO:CD	2.83	0.41
1:A:41:PRO:HG3	1:A:97:LEU:HD11	2.02	0.41
1:A:224:ARG:HD3	1:A:487:GLY:CA	2.50	0.41
1:A:428:TYR:CD1	1:A:428:TYR:C	2.98	0.41
1:A:524:LEU:O	1:A:525:ARG:C	2.63	0.41
1:B:491:ASP:HB3	1:B:494:ASP:HB3	2.02	0.41
1:B:496:LYS:HE3	1:B:496:LYS:HB2	1.83	0.41
1:A:213:ILE:HD13	1:A:324:LEU:HD21	2.02	0.41
1:B:44:SER:HA	1:B:274:ARG:HD2	2.02	0.41
1:B:335:GLY:HA3	1:B:399:SER:O	2.21	0.41
1:B:433:ARG:NH2	1:B:439:TRP:O	2.53	0.41
1:B:534:ARG:HD3	6:B:769:HOH:O	2.20	0.41
1:A:440:PRO:HD2	1:A:443:MET:SD	2.61	0.41
1:B:295:PHE:CE2	1:B:338:PHE:CZ	3.08	0.41
1:A:251:LEU:O	1:A:251:LEU:HG	2.09	0.41
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.92	0.41
1:B:200:PHE:CB	1:B:226:VAL:HB	2.49	0.41
1:B:203[B]:SXE:H2C1	2:B:601:HI6:C4	2.50	0.41
1:B:107:ARG:O	1:B:108:PRO:C	2.63	0.41
1:B:195:MET:C	1:B:223:HIS:CE1	2.99	0.41
1:B:375:ALA:O	1:B:379:VAL:HG23	2.21	0.41
1:B:101:VAL:HG22	1:B:147:VAL:HG22	2.03	0.41
1:A:99:LEU:C	1:A:99:LEU:HD12	2.46	0.40
1:A:286:TRP:CZ2	2:A:601:HI6:C8	3.01	0.40
1:B:203[B]:SXE:H2C1	2:B:601:HI6:H4	2.03	0.40
1:B:209:VAL:CG1	1:B:225:ALA:HB1	2.50	0.40
1:A:7:GLN:NE2	1:A:106:PRO:HB3	2.37	0.40
1:B:324:LEU:HD12	1:B:324:LEU:HA	1.77	0.40
1:A:294:ILE:HD11	1:A:402:VAL:HG21	2.04	0.40
1:B:316:ILE:O	1:B:421:GLN:NE2	2.54	0.40
1:B:495:SER:O	1:B:496:LYS:C	2.63	0.40
1:A:203[B]:SXE:H2C3	1:A:338:PHE:CZ	2.57	0.40
1:A:538:LYS:C	1:A:540:LEU:N	2.79	0.40
1:B:53:LYS:HG3	1:B:54:ARG:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HB	1:B:197:VAL:HG22	2.04	0.40
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.55	0.40
1:B:457:LEU:N	1:B:458:PRO:HD2	2.35	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	535/548 (98%)	505 (94%)	24 (4%)	6 (1%)	11	29
1	B	528/548 (96%)	500 (95%)	21 (4%)	7 (1%)	9	25
All	All	1063/1096 (97%)	1005 (94%)	45 (4%)	13 (1%)	10	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	541	SER
1	A	544	ALA
1	A	545	THR
1	B	494	ASP
1	B	496	LYS
1	B	542	ALA
1	A	319	GLY
1	B	497	SER
1	B	541	SER
1	A	493	ARG
1	B	342	GLY
1	B	121	GLY

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	443/445 (100%)	421 (95%)	22 (5%)	22	48
1	B	437/445 (98%)	412 (94%)	25 (6%)	18	43
All	All	880/890 (99%)	833 (95%)	47 (5%)	20	46

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	13	ARG
1	A	21	ARG
1	A	23	LYS
1	A	45	ARG
1	A	66	GLN
1	A	70	TYR
1	A	110	SER
1	A	118	ILE
1	A	224	ARG
1	A	246	ARG
1	A	322	GLN
1	A	332	LYS
1	A	340	VAL
1	A	350	ASN
1	A	369	GLN
1	A	413	GLN
1	A	421	GLN
1	A	441	LEU
1	A	524	LEU
1	A	536	LEU
1	B	9	LEU
1	B	23	LYS
1	B	66	GLN
1	B	94	GLU
1	B	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	ARG
1	B	166	GLU
1	B	181	GLN
1	B	216	LEU
1	B	239	VAL
1	B	246	ARG
1	B	265	ASN
1	B	291	GLN
1	B	296	ARG
1	B	327	LEU
1	B	340	VAL
1	B	350	ASN
1	B	360	LEU
1	B	369	GLN
1	B	376	GLU
1	B	421	GLN
1	B	437	LEU
1	B	505	THR
1	B	514	ASN
1	B	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	66	GLN
1	A	100	ASN
1	A	176	GLN
1	A	181	GLN
1	A	186	ASN
1	A	317	ASN
1	A	350	ASN
1	A	393	HIS
1	A	421	GLN
1	A	474	GLN
1	B	7	GLN
1	B	66	GLN
1	B	71	GLN
1	B	150	ASN
1	B	228	GLN
1	B	291	GLN
1	B	350	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	GLN
1	B	369	GLN
1	B	387	HIS
1	B	421	GLN
1	B	514	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SXE	B	203[A]	1	13,14,15	1.48	1 (7%)	14,18,20	0.90	0
1	SXE	B	203[B]	1	13,14,15	1.47	1 (7%)	14,18,20	1.01	1 (7%)
1	SXE	A	203[A]	1	13,14,15	1.49	1 (7%)	14,18,20	1.24	2 (14%)
1	SXE	A	203[B]	1	13,14,15	1.47	1 (7%)	14,18,20	1.01	1 (7%)

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
1	SXE	B	203[A]	1	-	7/15/17/19	-
1	SXE	B	203[B]	1	-	4/15/17/19	-
1	SXE	A	203[A]	1	-	8/15/17/19	-
1	SXE	A	203[B]	1	-	9/15/17/19	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203[A]	SXE	P1-N1	4.27	1.67	1.61
1	A	203[B]	SXE	P1-N1	4.24	1.67	1.61
1	B	203[B]	SXE	P1-N1	4.23	1.66	1.61
1	B	203[A]	SXE	P1-N1	4.23	1.66	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203[A]	SXE	P1-N1-C1	-3.31	119.67	125.03
1	A	203[A]	SXE	O2-P1-N1	-2.08	103.60	108.00
1	A	203[B]	SXE	O2-P1-N1	-2.04	103.70	108.00
1	B	203[B]	SXE	P1-N1-C1	-2.01	121.78	125.03

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203[A]	SXE	N-CA-CB-OG
1	A	203[A]	SXE	CB-OG-P1-N1
1	A	203[A]	SXE	C1-N1-P1-O1
1	A	203[B]	SXE	N-CA-CB-OG
1	A	203[B]	SXE	C4-O2-P1-O1
1	B	203[A]	SXE	N-CA-CB-OG
1	B	203[A]	SXE	CB-OG-P1-N1
1	B	203[A]	SXE	C1-N1-P1-O1
1	B	203[B]	SXE	N-CA-CB-OG
1	A	203[A]	SXE	CB-OG-P1-O1
1	A	203[B]	SXE	CB-OG-P1-O1
1	B	203[A]	SXE	CB-OG-P1-O1
1	B	203[B]	SXE	CB-OG-P1-O1
1	A	203[B]	SXE	C4-O2-P1-N1
1	A	203[B]	SXE	CB-OG-P1-O2
1	B	203[A]	SXE	C4-O2-P1-OG
1	B	203[B]	SXE	CB-OG-P1-O2
1	A	203[A]	SXE	C4-O2-P1-OG
1	A	203[B]	SXE	C4-O2-P1-OG
1	A	203[B]	SXE	C3-C1-N1-P1
1	A	203[B]	SXE	C2-C1-N1-P1
1	B	203[B]	SXE	CB-OG-P1-N1
1	B	203[A]	SXE	C4-O2-P1-N1
1	A	203[A]	SXE	CB-OG-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	203[A]	SXE	C4-O2-P1-N1
1	A	203[A]	SXE	C4-O2-P1-O1
1	B	203[A]	SXE	CB-OG-P1-O2
1	A	203[B]	SXE	CB-OG-P1-N1

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	203[A]	SXE	1	0
1	B	203[B]	SXE	3	0
1	A	203[A]	SXE	5	0
1	A	203[B]	SXE	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	CO3	B	602	-	3,3,3	0.95	0	2,3,3	0.45	0
3	NAG	A	603	1	14,14,15	0.75	0	17,19,21	1.85	2 (11%)
4	P6G	A	604	-	18,18,18	1.78	5 (27%)	17,17,17	2.16	11 (64%)
2	HI6	A	601	-	17,19,22	0.61	0	17,24,28	0.88	0
5	CO3	A	605	-	3,3,3	1.15	0	2,3,3	0.80	0
2	HI6	B	601	-	17,19,22	0.55	0	17,24,28	0.83	0
3	NAG	A	602	-	14,14,15	0.54	0	17,19,21	2.00	3 (17%)

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	NAG	A	603	1	1/1/5/7	1/6/23/26	0/1/1/1
4	P6G	A	604	-	-	7/16/16/16	-
2	HI6	A	601	-	-	3/10/10/13	0/2/2/2
2	HI6	B	601	-	-	4/10/10/13	0/2/2/2
3	NAG	A	602	-	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	P6G	C15-C14	-2.92	1.34	1.49
4	A	604	P6G	C6-C5	-2.88	1.34	1.49
4	A	604	P6G	C9-C8	-2.86	1.34	1.49
4	A	604	P6G	C17-C18	-2.85	1.34	1.49
4	A	604	P6G	C3-C2	-2.84	1.34	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C1-O5-C5	5.36	119.37	112.19
3	A	602	NAG	C1-C2-N2	-4.93	102.67	110.43
3	A	602	NAG	O5-C1-C2	4.22	117.82	111.29
3	A	603	NAG	C1-C2-N2	-3.87	104.33	110.43
4	A	604	P6G	O7-C8-C9	3.43	125.97	110.35
3	A	602	NAG	C1-O5-C5	3.39	116.73	112.19
4	A	604	P6G	O7-C6-C5	2.78	123.03	110.35
4	A	604	P6G	O13-C14-C15	2.74	122.85	110.35
4	A	604	P6G	O16-C15-C14	2.50	121.75	110.35
4	A	604	P6G	C5-O4-C3	2.49	124.17	113.26
4	A	604	P6G	O10-C9-C8	2.49	121.71	110.35
4	A	604	P6G	O16-C17-C18	2.34	120.42	110.11
4	A	604	P6G	O4-C3-C2	2.14	119.54	110.11
4	A	604	P6G	O4-C5-C6	2.06	119.74	110.35
4	A	604	P6G	C11-O10-C9	2.03	122.14	113.26
4	A	604	P6G	C17-O16-C15	2.03	122.13	113.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	603	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HI6	O2-C7-N2-C6
2	B	601	HI6	O2-C8-N3-C9
2	B	601	HI6	O2-C8-N3-C13
2	B	601	HI6	O2-C7-N2-C6
3	A	602	NAG	C4-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
4	A	604	P6G	O13-C14-C15-O16
4	A	604	P6G	O4-C5-C6-O7
4	A	604	P6G	O7-C8-C9-O10
4	A	604	P6G	C14-C15-O16-C17
4	A	604	P6G	C6-C5-O4-C3
2	B	601	HI6	N3-C8-O2-C7
4	A	604	P6G	C18-C17-O16-C15
2	A	601	HI6	N2-C7-O2-C8
3	A	602	NAG	C1-C2-N2-C7
2	A	601	HI6	N3-C8-O2-C7
4	A	604	P6G	C12-C11-O10-C9
3	A	603	NAG	C4-C5-C6-O6

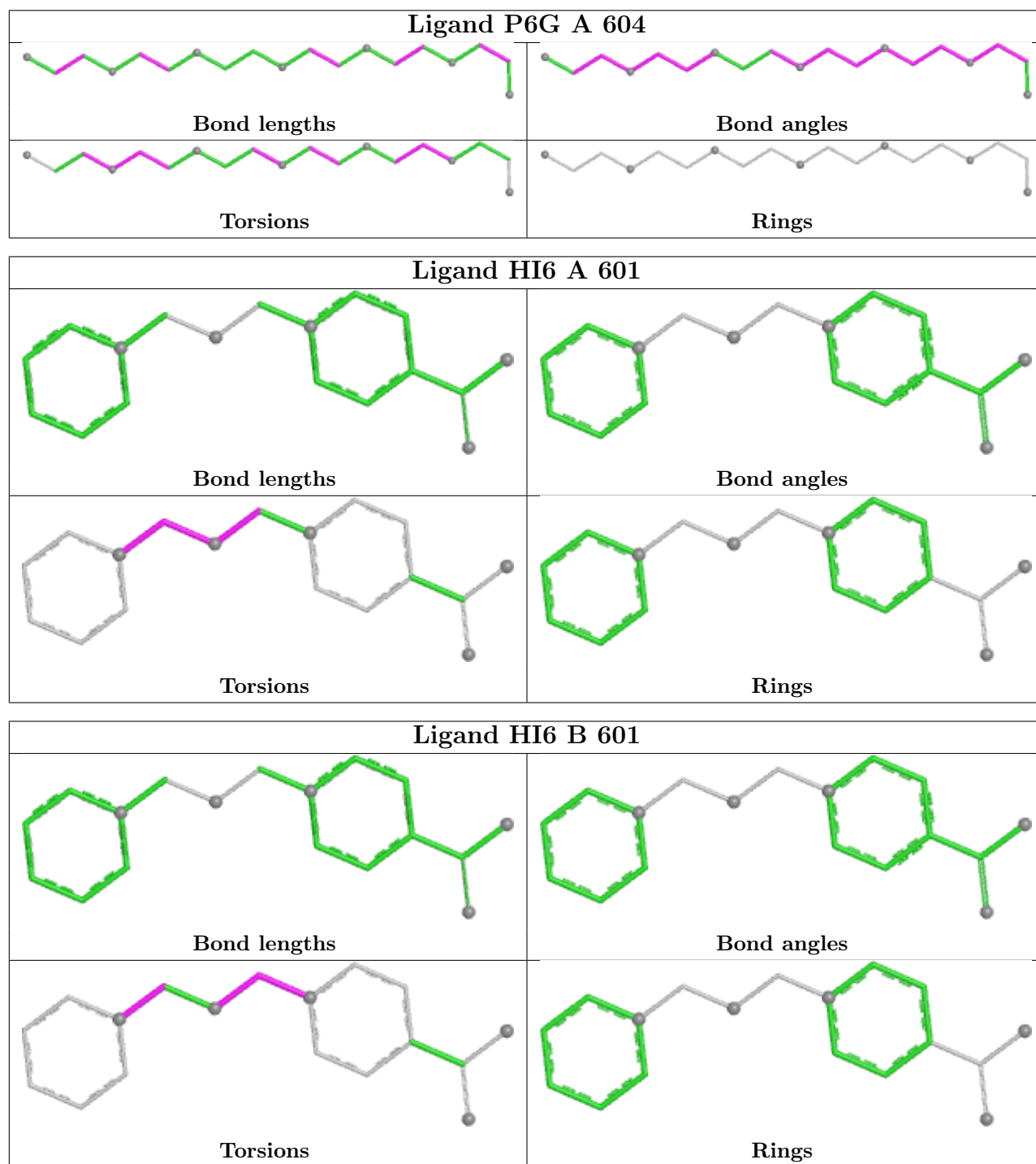
There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	P6G	4	0
2	A	601	HI6	11	0
2	B	601	HI6	9	0
3	A	602	NAG	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	538/548 (98%)	-0.86	2 (0%) 88 87	29, 45, 83, 159	1 (0%)
1	B	532/548 (97%)	-0.76	3 (0%) 85 85	29, 52, 85, 145	0
All	All	1070/1096 (97%)	-0.81	5 (0%) 87 86	29, 48, 84, 159	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	3.9
1	B	496	LYS	3.1
1	A	257	CYS	2.8
1	A	544	ALA	2.6
1	B	543	THR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SXE	B	203[A]	15/16	0.97	0.09	37,54,64,67	15
1	SXE	B	203[B]	15/16	0.97	0.09	37,52,64,66	15
1	SXE	A	203[A]	15/16	0.98	0.08	32,39,55,58	15
1	SXE	A	203[B]	15/16	0.98	0.08	30,38,54,58	15

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

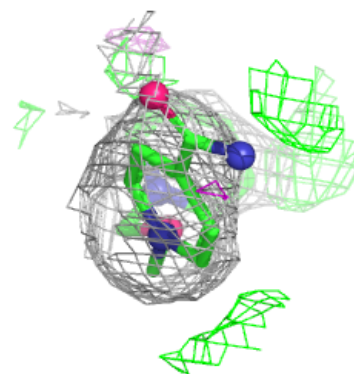
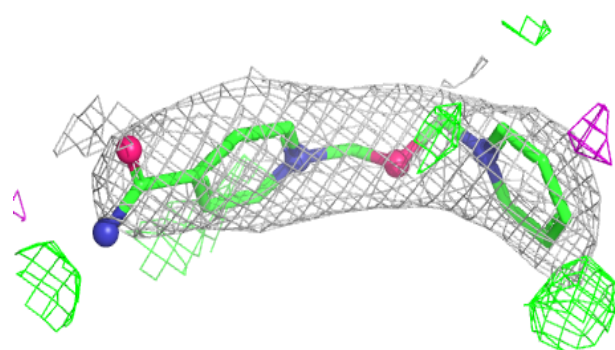
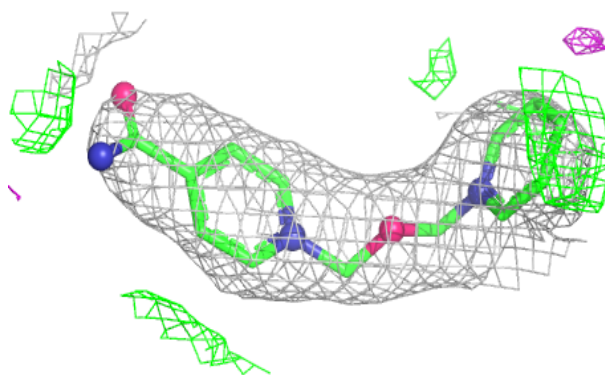
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	603	14/15	0.79	0.13	106,119,126,126	0
5	CO3	A	605	4/4	0.83	0.13	78,82,82,86	0
3	NAG	A	602	14/15	0.84	0.15	87,110,117,118	0
5	CO3	B	602	4/4	0.89	0.10	87,87,94,98	0
2	HI6	B	601	18/21	0.91	0.16	78,93,106,108	0
2	HI6	A	601	18/21	0.94	0.12	56,71,88,89	0
4	P6G	A	604	19/19	0.95	0.14	46,81,100,100	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.

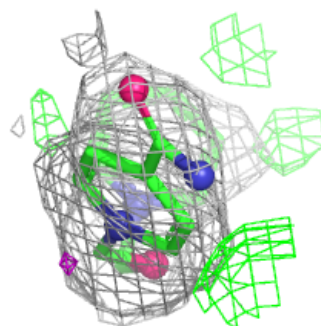
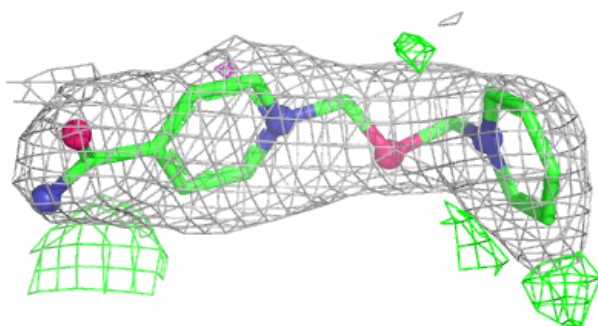
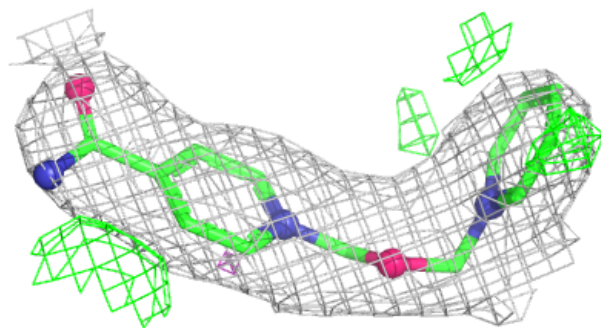
Electron density around HI6 B 601:

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



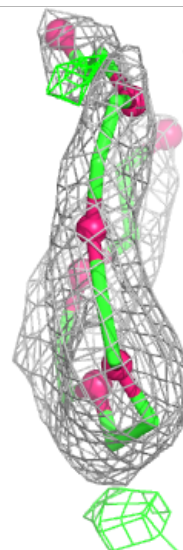
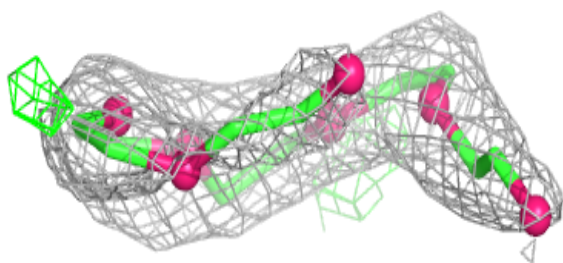
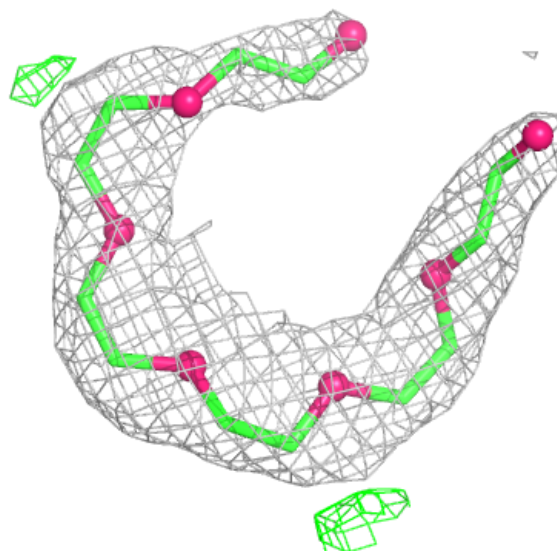
Electron density around HI6 A 601:

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



Electron density around P6G A 604:

$2mF_o-DF_c$ (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.