



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:13 PM UTC

PDB ID : 6G4O / pdb_00006g4o
Title : Non-aged form of Torpedo californica acetylcholinesterase inhibited by tabun analog NEDPA bound to uncharged reactivator 1
Authors : Santoni, G.; De la Mora, E.; de Souza, J.; Silman, I.; Sussman, J.; Baati, R.; Weik, M.; Nachon, F.
Deposited on : 2018-03-28
Resolution : 2.78 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

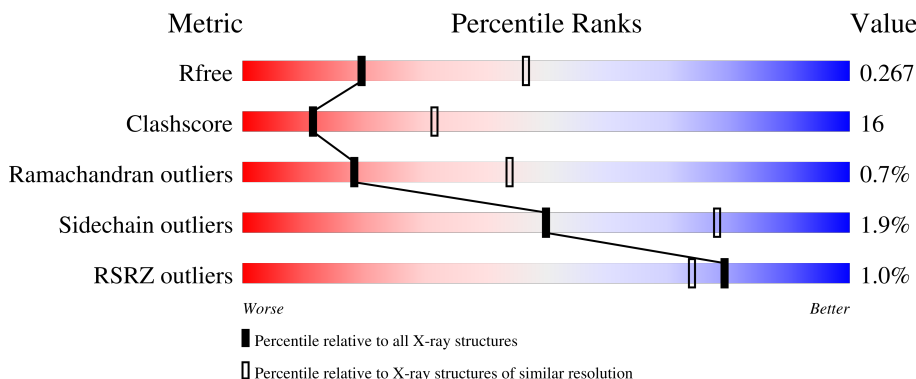
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	537	2% 66% 31% ..
1	B	537	66% 31% ..

2 Entry composition [i](#)

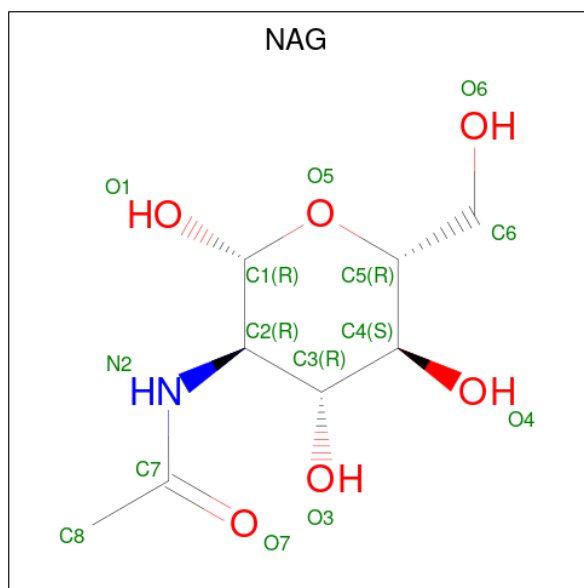
There are 9 unique types of molecules in this entry. The entry contains 8856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	528	Total	C	N	O	S	0	1	0
			4215	2706	713	773	23			
1	B	532	Total	C	N	O	S	0	1	0
			4252	2726	723	781	22			

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



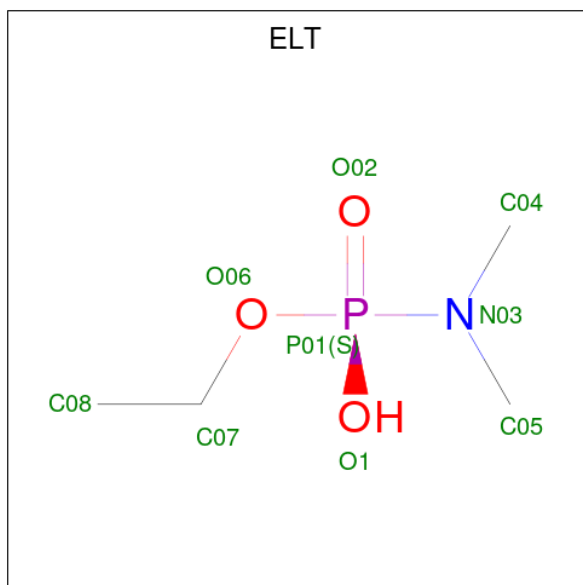
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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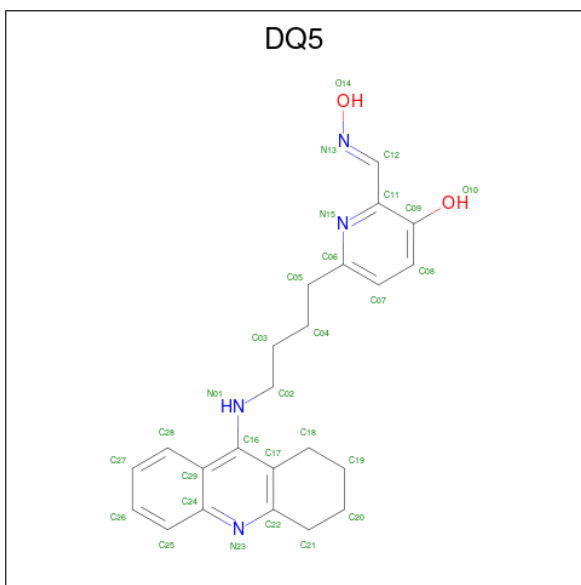
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ethoxy- {N}, {N}-dimethyl-phosphonamidic acid (CCD ID: ELT) (formula: $C_4H_{12}NO_3P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
3	B	1	Total	C	N	O	P	0	0
			8	4	1	2	1		

- Molecule 4 is 2-[({E})-hydroxyiminomethyl]-6-[4-(1,2,3,4-tetrahydroacridin-9-ylamino)butyl]pyridin-3-ol (CCD ID: DQ5) (formula: $C_{23}H_{26}N_4O_2$).

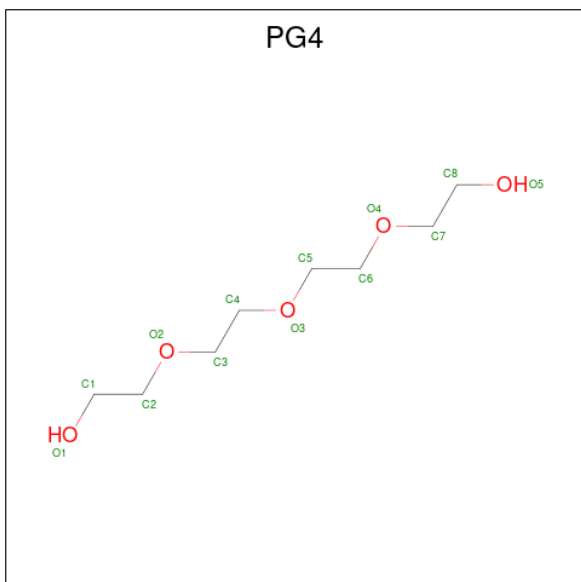


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	23	4	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Cl	0	0
			5	5		
5	B	3	Total	Cl	0	0
			3	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).

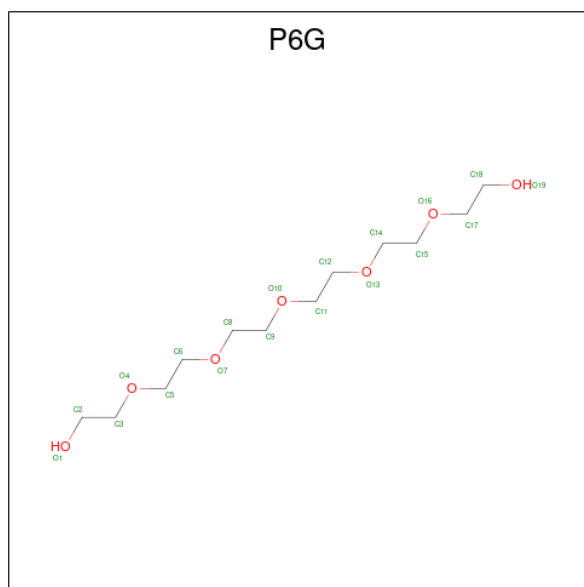


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Na		0	0
			1	1			

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			19	12	7		

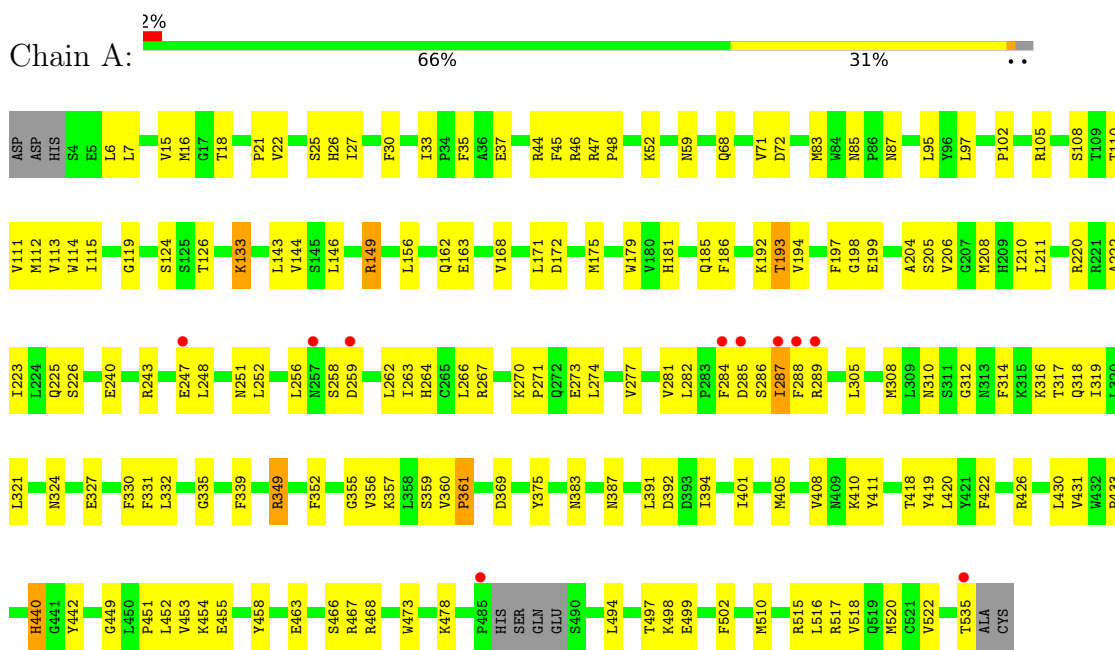
- Molecule 9 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	107	Total	O		0	0
			107	107			
9	B	126	Total	O		0	0
			126	126			

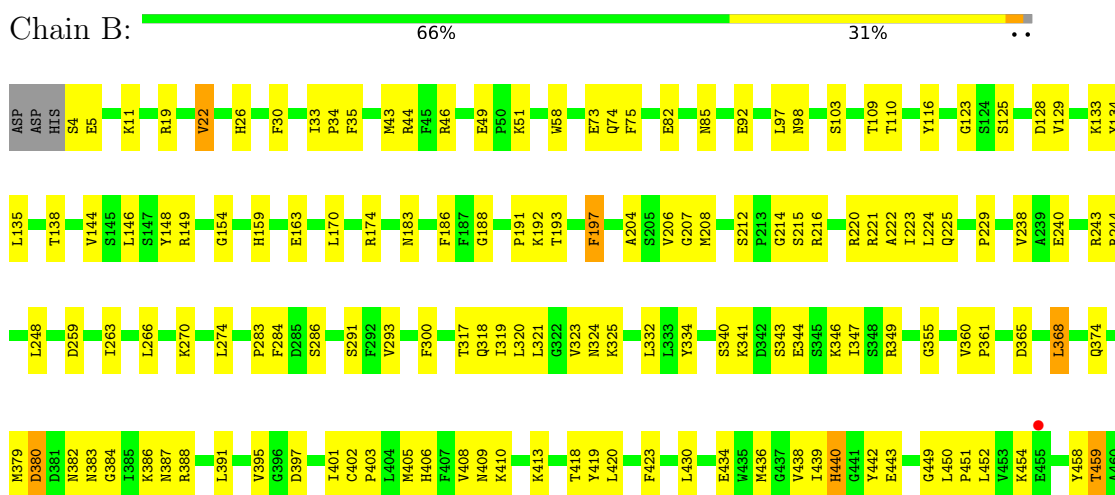
3 Residue-property plots [i](#)

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	91.54Å 106.35Å 150.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.98 – 2.78 45.98 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.98-2.78) 98.6 (45.98-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.264 0.191 , 0.267	Depositor DCC
R_{free} test set	1864 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	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	8856	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 37.71 % 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 4.1180e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DQ5, NA, P6G, ELT, NAG, PG4, CL

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	0.36	0/4339	0.61	0/5889
1	B	0.39	0/4378	0.64	1/5943 (0.0%)
All	All	0.38	0/8717	0.62	1/11832 (0.0%)

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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	499	GLU	N-CA-C	-6.30	103.94	113.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	286	SER	Peptide
1	B	498	LYS	Peptide

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	4215	0	4077	132	2
1	B	4252	0	4107	140	2
2	A	28	0	26	0	0
2	B	42	0	39	0	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
4	A	29	0	0	0	0
5	A	5	0	0	1	0
5	B	3	0	0	0	0
6	A	13	0	18	1	0
7	B	1	0	0	0	0
8	B	19	0	26	3	0
9	A	107	0	0	12	0
9	B	126	0	0	17	0
All	All	8856	0	8293	271	2

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 16.

All (271) 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:397:ASP:OD1	1:B:517:ARG:NH1	2.00	0.94
1:A:310:ASN:OD1	1:A:410:LYS:NZ	2.03	0.91
1:B:487:SER:O	1:B:491:LYS:NZ	2.13	0.81
1:B:473:TRP:O	9:B:701:HOH:O	1.99	0.79
1:B:125:SER:O	9:B:702:HOH:O	2.00	0.79
1:B:402:CYS:SG	9:B:763:HOH:O	2.40	0.79
1:B:174:ARG:NH1	1:B:214:GLY:C	2.42	0.78
1:B:483:ASN:HD21	1:B:492:TRP:H	1.30	0.77
1:A:369:ASP:OD1	1:B:530:LYS:NZ	2.18	0.76
1:A:463:GLU:OE2	1:A:467:ARG:NH1	2.18	0.75
1:A:37:GLU:OE2	1:A:52:LYS:N	2.19	0.75
1:A:375:TYR:OH	1:A:520:MET:HG2	1.88	0.74
1:A:312:GLY:O	1:A:316:LYS:NZ	2.22	0.72
1:A:339:PHE:O	9:A:701:HOH:O	2.06	0.72
1:A:168:VAL:HA	1:A:171:LEU:HD12	1.72	0.71
1:B:4:SER:N	9:B:708:HOH:O	2.24	0.69
1:A:451:PRO:HG2	1:A:466:SER:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TRP:NE1	9:B:707:HOH:O	2.23	0.68
1:B:159:HIS:HB3	1:B:238:VAL:HG13	1.77	0.67
1:A:248:LEU:HD21	1:A:274:LEU:HD23	1.75	0.67
1:B:324:ASN:ND2	1:B:443:GLU:OE1	2.19	0.66
1:A:108:SER:N	9:A:702:HOH:O	2.17	0.65
1:B:325:LYS:HB3	1:B:438:VAL:HG22	1.78	0.65
1:B:379:MET:HG3	9:B:709:HOH:O	1.94	0.65
1:A:285:ASP:O	1:A:287:ILE:N	2.27	0.65
1:B:365:ASP:HA	1:B:368:LEU:HD12	1.79	0.65
1:B:501:LYS:NZ	9:B:710:HOH:O	2.30	0.64
1:B:270:LYS:NZ	9:B:711:HOH:O	2.31	0.64
1:B:317:THR:HG22	1:B:318:GLN:H	1.63	0.64
1:B:405:MET:HA	1:B:408:VAL:HG12	1.79	0.63
1:A:452:LEU:HA	1:A:463:GLU:HG3	1.81	0.63
1:B:221:ARG:NH1	1:B:318:GLN:OE1	2.32	0.62
1:B:197:PHE:HB3	1:B:223:ILE:HB	1.81	0.62
1:B:225:GLN:NE2	1:B:473:TRP:HZ3	1.98	0.62
1:B:346:LYS:HB3	1:B:384:GLY:HA3	1.80	0.62
1:B:323:VAL:HG21	1:B:401:ILE:HD13	1.82	0.62
1:B:406:HIS:O	1:B:410:LYS:HG2	1.99	0.62
1:B:452:LEU:HD22	1:B:463:GLU:HG3	1.82	0.62
1:B:43:MET:HE1	1:B:49:GLU:HG3	1.81	0.62
1:A:430:LEU:HD11	1:A:442:TYR:CD2	2.35	0.61
1:B:46:ARG:HD3	1:B:163:GLU:OE2	2.00	0.61
1:B:11:LYS:H	1:B:183:ASN:ND2	1.99	0.60
1:B:499:GLU:O	1:B:514:GLN:NE2	2.34	0.60
1:B:19:ARG:NH1	1:B:103:SER:OG	2.35	0.60
1:A:44:ARG:NH1	1:A:266:LEU:O	2.35	0.59
1:A:405:MET:HA	1:A:408:VAL:HG12	1.84	0.59
1:A:426:ARG:NH1	1:A:433:PRO:O	2.35	0.59
1:A:226:SER:OG	1:A:327:GLU:OE2	2.20	0.59
1:B:30:PHE:HB3	1:B:33:ILE:HD11	1.85	0.59
1:A:357:LYS:NZ	9:A:708:HOH:O	2.36	0.58
1:B:240:GLU:O	1:B:244:ARG:HG3	2.04	0.58
1:B:380:ASP:OD2	1:B:386:LYS:NZ	2.32	0.58
1:B:408:VAL:HG23	1:B:418:THR:HG21	1.85	0.57
1:B:248:LEU:HD21	1:B:274:LEU:HD23	1.87	0.57
1:B:434:GLU:OE1	1:B:434:GLU:N	2.33	0.57
1:B:110:THR:OG1	1:B:478:LYS:HG2	2.03	0.57
1:B:483:ASN:ND2	1:B:492:TRP:H	2.01	0.57
1:A:324:ASN:HD22	1:A:440:HIS:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PHE:CB	1:B:223:ILE:HB	2.35	0.56
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.87	0.56
1:A:251:ASN:HB3	1:A:277:VAL:HG11	1.88	0.56
1:A:21:PRO:O	1:A:133:LYS:HE3	2.05	0.56
1:A:240:GLU:OE2	1:A:243:ARG:NH1	2.39	0.56
1:B:485:PRO:O	1:B:486:HIS:HB3	2.04	0.56
1:A:515:ARG:HA	9:A:752:HOH:O	2.06	0.56
1:A:247:GLU:OE1	1:A:281:VAL:HG12	2.07	0.55
1:A:383:ASN:C	1:A:383:ASN:HD22	2.14	0.55
1:B:498:LYS:HG2	1:B:500:GLN:HG3	1.87	0.55
1:A:468:ARG:HD3	9:A:714:HOH:O	2.05	0.55
1:A:463:GLU:O	1:A:467:ARG:HG3	2.07	0.55
1:A:35:PHE:CD2	1:A:97:LEU:HD23	2.41	0.54
1:B:5:GLU:HB2	9:B:764:HOH:O	2.06	0.54
1:B:347:ILE:HG12	1:B:388:ARG:HB2	1.89	0.54
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.89	0.54
1:A:240:GLU:OE1	1:A:243:ARG:HD3	2.08	0.54
1:B:225:GLN:NE2	1:B:473:TRP:CZ3	2.75	0.54
1:A:113:VAL:HG22	1:A:144:VAL:HB	1.88	0.54
1:B:44:ARG:NH2	1:B:92:GLU:OE2	2.29	0.54
1:B:293:VAL:O	9:B:704:HOH:O	2.18	0.54
1:B:284:PHE:CD2	1:B:361:PRO:HB2	2.43	0.54
1:B:109:THR:HG22	1:B:188:GLY:O	2.09	0.53
1:A:286:SER:C	1:A:288:PHE:H	2.16	0.53
1:B:134:TYR:O	1:B:138:THR:HG23	2.08	0.53
1:B:244:ARG:NH1	1:B:291:SER:O	2.38	0.53
1:B:191:PRO:HG3	9:B:726:HOH:O	2.09	0.53
1:B:332:LEU:HD21	1:B:395:VAL:HG21	1.91	0.53
1:A:286:SER:OG	1:A:289:ARG:HG2	2.08	0.53
1:B:344:GLU:OE1	1:B:346:LYS:NZ	2.42	0.53
1:B:474:ALA:O	1:B:478:LYS:HG3	2.09	0.53
1:A:47:ARG:NH1	1:A:162:GLN:OE1	2.40	0.53
1:B:135:LEU:HA	1:B:470:MET:HE2	1.90	0.53
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.91	0.52
1:B:43:MET:HE3	1:B:46:ARG:NH2	2.24	0.52
1:B:243:ARG:NH2	1:B:283:PRO:HG3	2.24	0.52
1:B:174:ARG:HH12	1:B:214:GLY:C	2.17	0.52
1:B:406:HIS:ND1	9:B:713:HOH:O	2.34	0.52
1:A:426:ARG:NH2	9:A:719:HOH:O	2.43	0.52
1:A:349:ARG:HH21	1:A:387:ASN:HD21	1.56	0.52
1:B:35:PHE:CD2	1:B:97:LEU:HD23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLN:NE2	1:A:473:TRP:HE1	2.08	0.51
1:A:391:LEU:HA	1:A:394:ILE:HD12	1.91	0.51
1:A:319:ILE:HD12	1:A:321:LEU:HD22	1.93	0.51
1:A:45:PHE:CE1	1:A:156:LEU:HD13	2.46	0.51
1:B:438:VAL:HG23	1:B:438:VAL:O	2.11	0.51
1:A:105:ARG:NH1	1:A:186:PHE:O	2.44	0.51
1:A:282:LEU:HD22	1:A:289:ARG:HB2	1.92	0.51
1:B:229:PRO:O	9:B:705:HOH:O	2.19	0.51
1:A:112:MET:HB2	1:A:143:LEU:HD12	1.91	0.51
1:A:48:PRO:O	1:A:175:MET:HE1	2.11	0.51
1:A:520:MET:HE2	9:A:792:HOH:O	2.11	0.51
1:A:349:ARG:HH21	1:A:387:ASN:ND2	2.10	0.50
1:B:82:GLU:HA	1:B:85:ASN:HD22	1.76	0.50
1:B:223:ILE:HD11	9:B:701:HOH:O	2.12	0.50
1:B:498:LYS:HG2	1:B:500:GLN:HE21	1.75	0.50
1:B:110:THR:HG23	1:B:193:THR:HG22	1.94	0.50
1:B:502:PHE:CE2	1:B:516:LEU:HB2	2.47	0.50
1:A:181:HIS:HD2	9:A:738:HOH:O	1.94	0.50
1:A:498:LYS:HG3	1:A:499:GLU:HG3	1.93	0.50
1:B:43:MET:HE1	1:B:49:GLU:CG	2.42	0.50
1:A:518:VAL:O	1:A:522:VAL:HG23	2.12	0.50
1:A:449:GLY:HA2	1:A:466:SER:OG	2.12	0.50
1:B:397:ASP:CG	1:B:517:ARG:NH1	2.70	0.50
1:A:7:LEU:HB2	1:A:16:MET:HE3	1.93	0.49
1:B:340:SER:HB3	1:B:343:SER:HB3	1.93	0.49
1:A:27:ILE:HG22	1:A:102:PRO:HA	1.93	0.49
1:A:37:GLU:CD	1:A:52:LYS:HG3	2.37	0.49
1:A:420:LEU:HD23	1:A:502:PHE:HB3	1.93	0.49
1:B:51:LYS:HE3	9:B:759:HOH:O	2.12	0.49
1:A:258:SER:OG	1:A:259:ASP:N	2.45	0.49
1:B:355:GLY:HA3	1:B:391:LEU:HD11	1.95	0.49
1:A:7:LEU:HB2	1:A:16:MET:CE	2.41	0.49
1:A:263:ILE:HG22	1:A:267:ARG:NH1	2.27	0.49
1:A:422:PHE:CD2	1:A:516:LEU:HD11	2.48	0.49
1:A:95:LEU:HD11	1:A:172:ASP:OD2	2.12	0.49
1:A:264:HIS:CD2	5:A:610:CL:CL	3.03	0.49
1:A:535:THR:HG21	1:B:534:ALA:HB1	1.94	0.49
1:A:37:GLU:OE2	1:A:52:LYS:HG3	2.12	0.49
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.95	0.49
1:A:287:ILE:HG21	1:A:335:GLY:HA3	1.94	0.48
1:B:397:ASP:HA	1:B:401:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ASN:HB3	9:B:812:HOH:O	2.14	0.48
1:B:518:VAL:O	1:B:522:VAL:HG23	2.14	0.48
1:A:115:ILE:HG23	1:A:146:LEU:HD11	1.95	0.48
1:B:440:HIS:CE1	8:B:609:P6G:H171	2.48	0.48
1:A:375:TYR:CZ	1:A:520:MET:HG2	2.49	0.48
1:B:317:THR:HG22	1:B:318:GLN:OE1	2.13	0.48
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.49	0.48
1:A:211:LEU:HD22	1:A:308:MET:HE2	1.96	0.47
1:B:266:LEU:HD22	1:B:274:LEU:HD21	1.96	0.47
1:B:374:GLN:O	1:B:374:GLN:HG3	2.13	0.47
1:A:194:VAL:O	1:A:220:ARG:HB3	2.15	0.47
1:B:473:TRP:N	1:B:473:TRP:CD1	2.82	0.47
1:A:163:GLU:OE1	1:A:267:ARG:NH2	2.47	0.47
1:B:11:LYS:HB2	1:B:183:ASN:HD21	1.78	0.47
1:A:87:ASN:ND2	1:A:126:THR:O	2.26	0.47
1:A:197:PHE:CB	1:A:223:ILE:HB	2.45	0.47
1:B:116:TYR:O	1:B:148:TYR:OH	2.29	0.47
1:B:360:VAL:HG12	1:B:360:VAL:O	2.15	0.47
1:B:469:ILE:O	1:B:473:TRP:CD1	2.68	0.47
1:A:46:ARG:O	1:A:149:ARG:NH2	2.39	0.47
1:A:284:PHE:HD1	1:A:361:PRO:HB3	1.81	0.46
1:B:135:LEU:HD13	1:B:470:MET:HE2	1.97	0.46
1:B:436:MET:HE2	1:B:439:ILE:HG12	1.97	0.46
1:B:19:ARG:NH2	1:B:26:HIS:HB2	2.29	0.46
1:B:498:LYS:HE3	1:B:515:ARG:CZ	2.45	0.46
1:A:72:ASP:H	1:A:85:ASN:HD21	1.63	0.46
1:A:453:VAL:HG12	1:A:455:GLU:HG2	1.97	0.46
1:A:119:GLY:N	3:A:603:ELT:O02	2.48	0.46
1:A:240:GLU:CD	1:A:243:ARG:HH11	2.23	0.46
1:A:270:LYS:HB2	1:A:273:GLU:HG3	1.98	0.46
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.50	0.46
1:B:270:LYS:HE2	1:B:270:LYS:HA	1.98	0.46
1:A:352:PHE:O	1:A:356:VAL:HG23	2.16	0.46
1:B:43:MET:HE2	1:B:43:MET:HB3	1.82	0.46
1:B:129:VAL:HA	1:B:450:LEU:HD11	1.97	0.46
1:A:68:GLN:HG3	1:A:271:PRO:HB3	1.98	0.46
1:B:374:GLN:HG3	1:B:520:MET:HE1	1.96	0.46
1:B:449:GLY:HA2	1:B:466:SER:OG	2.16	0.46
1:A:168:VAL:O	1:A:172:ASP:OD1	2.33	0.46
1:A:205:SER:HA	1:A:208:MET:CE	2.46	0.46
1:A:401:ILE:O	1:A:405:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:O	1:B:317:THR:HG21	2.16	0.46
1:B:349:ARG:HB2	1:B:382:ASN:OD1	2.16	0.46
1:B:498:LYS:O	9:B:706:HOH:O	2.21	0.46
1:A:317:THR:OG1	1:A:318:GLN:N	2.46	0.45
1:B:11:LYS:H	1:B:183:ASN:HD22	1.64	0.45
1:A:197:PHE:HB2	1:A:223:ILE:HB	1.99	0.45
1:B:383:ASN:O	1:B:387:ASN:ND2	2.49	0.45
1:A:211:LEU:HD13	1:A:305:LEU:HD22	1.98	0.45
1:B:222:ALA:HB3	1:B:319:ILE:HG22	1.99	0.45
1:A:22:VAL:HG11	1:A:27:ILE:HG13	1.99	0.45
1:A:263:ILE:CG2	1:A:267:ARG:NH1	2.80	0.45
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.74	0.45
1:A:401:ILE:HG21	1:A:517:ARG:HD3	1.98	0.45
1:A:502:PHE:CE1	1:A:516:LEU:HD12	2.51	0.45
1:A:331:PHE:CD1	1:A:331:PHE:N	2.85	0.45
1:A:454:LYS:HE3	9:A:749:HOH:O	2.17	0.45
1:A:431:VAL:HG22	9:A:794:HOH:O	2.17	0.45
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.47	0.44
1:A:27:ILE:HD11	1:A:133:LYS:HB2	1.98	0.44
1:B:413:LYS:HE2	1:B:413:LYS:HB3	1.65	0.44
1:A:408:VAL:HG23	1:A:418:THR:HG21	1.98	0.44
1:A:502:PHE:CZ	1:A:516:LEU:HD12	2.53	0.44
1:B:212:SER:O	1:B:216:ARG:HG3	2.18	0.44
1:A:360:VAL:HG23	1:A:360:VAL:O	2.17	0.44
1:A:240:GLU:HA	1:A:243:ARG:HG2	1.99	0.43
1:B:452:LEU:CD2	1:B:463:GLU:HG3	2.48	0.43
1:A:111:VAL:HG13	1:A:194:VAL:HA	2.00	0.43
1:B:22:VAL:HB	1:B:133:LYS:HD2	1.99	0.43
1:B:135:LEU:CD1	1:B:470:MET:HE2	2.48	0.43
1:B:149:ARG:O	1:B:154:GLY:HA3	2.19	0.43
1:B:174:ARG:NH1	1:B:214:GLY:O	2.51	0.43
1:B:223:ILE:HA	1:B:320:LEU:O	2.18	0.43
1:A:25:SER:OG	1:A:26:HIS:N	2.52	0.43
1:A:286:SER:O	1:A:288:PHE:N	2.51	0.43
1:B:402:CYS:N	1:B:403:PRO:HD2	2.34	0.43
1:A:6:LEU:O	1:A:16:MET:HA	2.18	0.43
1:A:193:THR:O	1:A:193:THR:OG1	2.36	0.43
1:A:284:PHE:CD1	1:A:361:PRO:HB3	2.54	0.43
1:B:34:PRO:HG3	1:B:58:TRP:CH2	2.54	0.43
1:B:221:ARG:NH1	1:B:480:GLY:HA3	2.33	0.43
1:B:459:THR:HG22	1:B:461:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:SER:HA	1:A:208:MET:HE2	2.00	0.43
1:A:270:LYS:HE3	1:A:270:LYS:HB3	1.81	0.43
1:B:75:PHE:CE2	1:B:341:LYS:HD3	2.53	0.43
1:B:420:LEU:HD23	1:B:502:PHE:CB	2.49	0.43
1:A:30:PHE:HB3	1:A:33:ILE:HD11	2.01	0.42
1:A:251:ASN:HB3	1:A:277:VAL:CG1	2.48	0.42
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.69	0.42
1:B:204:ALA:O	1:B:208:MET:HG3	2.20	0.42
1:B:430:LEU:HD21	1:B:442:TYR:CD2	2.55	0.42
1:B:454:LYS:HA	1:B:454:LYS:HD3	1.51	0.42
1:A:181:HIS:CD2	9:A:738:HOH:O	2.72	0.42
1:B:98:ASN:O	1:B:144:VAL:HA	2.19	0.42
1:B:221:ARG:HG2	1:B:221:ARG:HH11	1.84	0.42
1:B:11:LYS:HG3	1:B:186:PHE:HE2	1.85	0.42
1:B:116:TYR:CD1	1:B:123:GLY:HA3	2.55	0.42
1:B:193:THR:HG22	1:B:193:THR:O	2.19	0.42
1:A:179:TRP:HA	9:A:759:HOH:O	2.19	0.42
1:B:440:HIS:HE1	8:B:609:P6G:H171	1.85	0.42
8:B:609:P6G:H111	8:B:609:P6G:H142	1.67	0.42
1:A:332:LEU:HD11	1:A:392:ASP:HA	2.01	0.42
1:A:355:GLY:O	1:A:359:SER:N	2.38	0.42
1:B:206:VAL:CG1	1:B:224:LEU:HG	2.50	0.42
1:A:175:MET:HE3	1:A:175:MET:HB2	1.95	0.41
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.55	0.41
1:B:259:ASP:O	1:B:263:ILE:HG13	2.18	0.41
1:A:35:PHE:HD2	1:A:97:LEU:HD23	1.84	0.41
1:B:321:LEU:O	1:B:420:LEU:HA	2.20	0.41
1:A:114:TRP:CZ3	1:A:198:GLY:HA2	2.54	0.41
1:A:247:GLU:OE1	1:A:251:ASN:OD1	2.38	0.41
1:A:199:GLU:OE1	6:A:607:PG4:O1	2.32	0.41
1:A:408:VAL:CG2	1:A:418:THR:HG21	2.51	0.41
1:B:174:ARG:NH1	1:B:215:SER:N	2.69	0.41
1:B:324:ASN:OD1	1:B:423:PHE:HB3	2.20	0.41
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.90	0.41
1:B:243:ARG:HH22	1:B:283:PRO:HG3	1.85	0.41
1:A:110:THR:OG1	1:A:478:LYS:HG2	2.21	0.41
1:A:262:LEU:O	1:A:266:LEU:HG	2.21	0.41
1:A:319:ILE:HG12	1:A:411:TYR:CE2	2.56	0.41
1:A:510:MET:HE2	1:A:510:MET:HB3	1.87	0.41
1:B:125:SER:HB3	1:B:146:LEU:O	2.21	0.41
1:B:197:PHE:N	1:B:197:PHE:CD2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:O	1:A:208:MET:HG3	2.20	0.40
1:A:210:ILE:HD11	1:A:222:ALA:CB	2.51	0.40
1:B:43:MET:HE3	1:B:46:ARG:HH21	1.87	0.40
1:B:74:GLN:HG3	1:B:334:TYR:CD2	2.57	0.40
1:B:419:TYR:CZ	1:B:482:PRO:HD2	2.57	0.40
1:A:451:PRO:HG2	1:A:466:SER:CB	2.48	0.40
1:B:170:LEU:HD13	1:B:300:PHE:CE1	2.57	0.40
1:B:397:ASP:CG	1:B:517:ARG:HH11	2.28	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:O	1:B:192:LYS:NZ[2_554]	2.12	0.08
1:A:192:LYS:NZ	1:B:73:GLU:OE1[2_454]	2.13	0.07

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	525/537 (98%)	489 (93%)	33 (6%)	3 (1%)	21	47
1	B	531/537 (99%)	492 (93%)	35 (7%)	4 (1%)	16	40
All	All	1056/1074 (98%)	981 (93%)	68 (6%)	7 (1%)	18	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ILE
1	A	59	ASN
1	B	22	VAL
1	B	128	ASP

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Mol	Chain	Res	Type
1	B	380	ASP
1	B	515	ARG
1	A	361	PRO

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	462/469 (98%)	449 (97%)	13 (3%)	38	70
1	B	466/469 (99%)	461 (99%)	5 (1%)	65	85
All	All	928/938 (99%)	910 (98%)	18 (2%)	50	78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	18	THR
1	A	83	MET
1	A	124	SER
1	A	133	LYS
1	A	149	ARG
1	A	185	GLN
1	A	193	THR
1	A	256	LEU
1	A	330	PHE
1	A	349	ARG
1	A	440	HIS
1	A	497	THR
1	B	197	PHE
1	B	368	LEU
1	B	440	HIS
1	B	459	THR
1	B	497	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	66	ASN
1	A	68	GLN
1	A	85	ASN
1	A	159	HIS
1	A	181	HIS
1	A	225	GLN
1	A	251	ASN
1	A	253	ASN
1	A	324	ASN
1	A	383	ASN
1	A	387	ASN
1	A	525	ASN
1	B	9	ASN
1	B	66	ASN
1	B	85	ASN
1	B	162	GLN
1	B	178	GLN
1	B	183	ASN
1	B	253	ASN
1	B	272	GLN
1	B	364	ASN
1	B	409	ASN
1	B	483	ASN
1	B	500	GLN
1	B	513	HIS
1	B	514	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

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 for Mogul analysis.

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
8	P6G	B	609	-	18,18,18	0.70	0	17,17,17	1.13	0
2	NAG	A	601	1	14,14,15	0.99	1 (7%)	17,19,21	0.65	0
6	PG4	A	607	-	12,12,12	0.67	0	11,11,11	1.27	0
2	NAG	A	602	1	14,14,15	0.72	0	17,19,21	0.66	0
2	NAG	B	601	1	14,14,15	0.50	0	17,19,21	0.62	1 (5%)
3	ELT	A	603	1	4,7,8	1.83	2 (50%)	4,8,11	0.82	0
3	ELT	B	603	1	4,7,8	2.02	1 (25%)	4,8,11	1.06	0
4	DQ5	A	604	-	31,32,32	1.80	6 (19%)	36,43,43	1.50	7 (19%)
2	NAG	B	604	1	14,14,15	0.25	0	17,19,21	0.67	1 (5%)
2	NAG	B	602	1	14,14,15	0.46	0	17,19,21	0.72	1 (5%)

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
8	P6G	B	609	-	-	10/16/16/16	-
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	PG4	A	607	-	-	5/10/10/10	-
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	ELT	A	603	1	-	0/1/7/10	-
3	ELT	B	603	1	-	0/1/7/10	-
4	DQ5	A	604	-	-	8/11/18/18	0/4/4/4
2	NAG	B	604	1	-	2/6/23/26	0/1/1/1
2	NAG	B	602	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	DQ5	C22-N23	5.93	1.39	1.32
3	B	603	ELT	C04-N03	-3.56	1.40	1.45
2	A	601	NAG	O5-C1	3.38	1.49	1.43
4	A	604	DQ5	C16-C17	3.30	1.45	1.39
4	A	604	DQ5	C16-N01	3.17	1.46	1.37
4	A	604	DQ5	O10-C09	3.13	1.42	1.36
3	A	603	ELT	C05-N03	2.50	1.49	1.45
3	A	603	ELT	C04-N03	-2.43	1.42	1.45
4	A	604	DQ5	C12-N13	2.33	1.32	1.27
4	A	604	DQ5	C29-C24	-2.05	1.39	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	DQ5	O14-N13-C12	4.83	120.17	111.83
4	A	604	DQ5	C22-N23-C24	2.99	121.21	117.67
4	A	604	DQ5	C17-C22-N23	-2.64	121.80	123.66
4	A	604	DQ5	C29-C24-N23	-2.59	120.06	122.80
4	A	604	DQ5	C21-C22-C17	2.38	123.83	121.40
4	A	604	DQ5	C25-C24-C29	2.36	121.67	119.13
2	B	604	NAG	C1-O5-C5	2.35	115.34	112.19
2	B	602	NAG	C1-O5-C5	2.27	115.22	112.19
4	A	604	DQ5	C05-C06-N15	2.12	119.27	116.06
2	B	601	NAG	C1-O5-C5	2.07	114.97	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	DQ5	C09-C11-C12-N13
4	A	604	DQ5	N15-C11-C12-N13
2	B	601	NAG	O5-C5-C6-O6
2	B	601	NAG	C4-C5-C6-O6
2	A	602	NAG	O5-C5-C6-O6
2	B	604	NAG	C4-C5-C6-O6
4	A	604	DQ5	C02-C03-C04-C05
6	A	607	PG4	O3-C5-C6-O4
8	B	609	P6G	O16-C17-C18-O19
2	A	602	NAG	C4-C5-C6-O6
2	B	604	NAG	O5-C5-C6-O6
6	A	607	PG4	O4-C7-C8-O5

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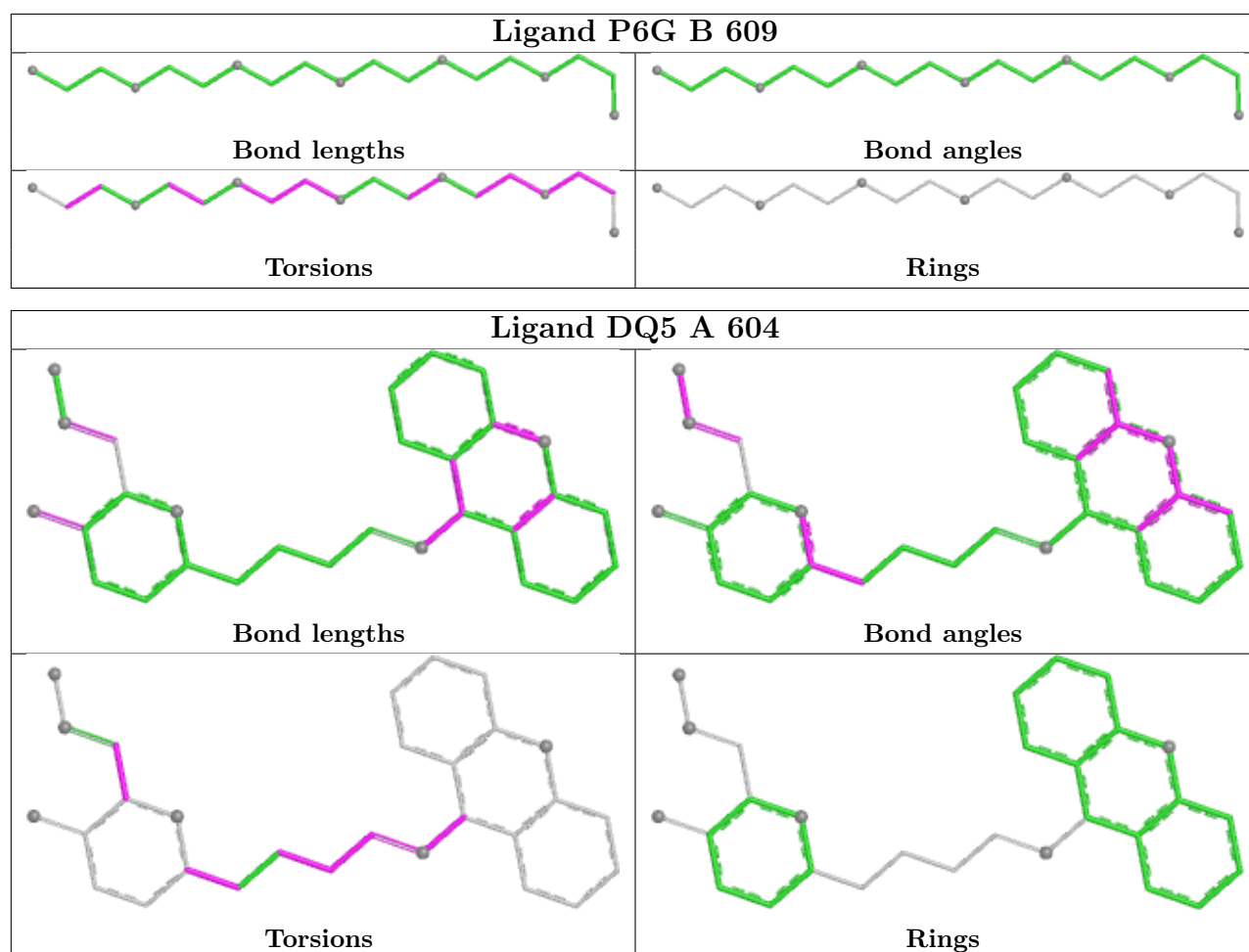
Mol	Chain	Res	Type	Atoms
8	B	609	P6G	O10-C11-C12-O13
4	A	604	DQ5	N01-C02-C03-C04
8	B	609	P6G	O13-C14-C15-O16
2	B	602	NAG	C4-C5-C6-O6
6	A	607	PG4	O1-C1-C2-O2
2	B	602	NAG	O5-C5-C6-O6
4	A	604	DQ5	C03-C02-N01-C16
4	A	604	DQ5	C04-C05-C06-C07
6	A	607	PG4	C6-C5-O3-C4
8	B	609	P6G	C9-C8-O7-C6
4	A	604	DQ5	C29-C16-N01-C02
8	B	609	P6G	O1-C2-C3-O4
6	A	607	PG4	O2-C3-C4-O3
8	B	609	P6G	C2-C3-O4-C5
8	B	609	P6G	C11-C12-O13-C14
4	A	604	DQ5	C04-C05-C06-N15
8	B	609	P6G	C12-C11-O10-C9
8	B	609	P6G	C6-C5-O4-C3
8	B	609	P6G	O4-C5-C6-O7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	609	P6G	3	0
6	A	607	PG4	1	0
3	A	603	ELT	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 [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	528/537 (98%)	0.01	10 (1%) 66 59	30, 52, 87, 147	1 (0%)
1	B	532/537 (99%)	-0.18	1 (0%) 91 89	24, 46, 73, 136	1 (0%)
All	All	1060/1074 (98%)	-0.09	11 (1%) 79 74	24, 49, 79, 147	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	3.3
1	A	485	PRO	3.2
1	A	287	ILE	2.9
1	A	535	THR	2.5
1	A	247	GLU	2.5
1	A	288	PHE	2.4
1	A	259	ASP	2.4
1	B	455	GLU	2.3
1	A	285	ASP	2.3
1	A	257	ASN	2.0
1	A	289	ARG	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

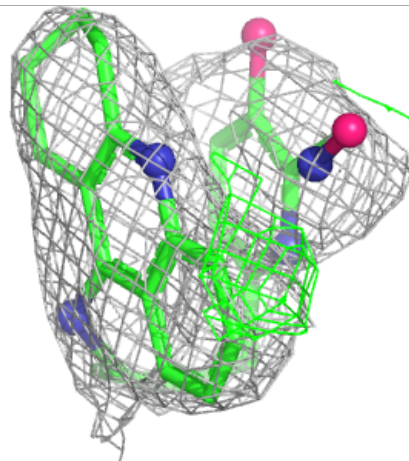
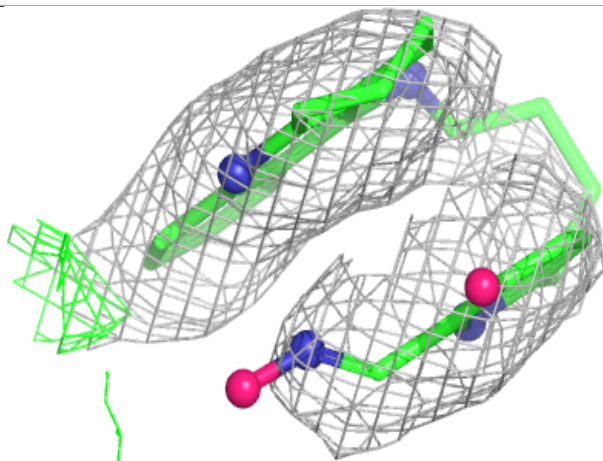
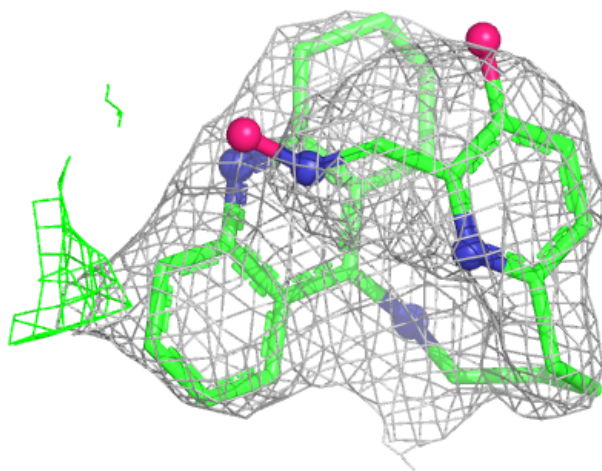
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CL	A	610	1/1	0.69	0.16	86,86,86,86	0
2	NAG	B	604	14/15	0.70	0.12	68,92,101,101	0
2	NAG	A	601	14/15	0.77	0.13	67,79,87,89	0
2	NAG	B	601	14/15	0.78	0.12	80,95,101,102	0
2	NAG	B	602	14/15	0.78	0.11	43,66,81,82	0
5	CL	A	609	1/1	0.85	0.13	81,81,81,81	0
2	NAG	A	602	14/15	0.85	0.09	42,55,79,82	0
5	CL	B	607	1/1	0.88	0.14	83,83,83,83	0
5	CL	A	605	1/1	0.89	0.15	77,77,77,77	0
6	PG4	A	607	13/13	0.89	0.15	49,57,63,64	0
7	NA	B	606	1/1	0.90	0.10	63,63,63,63	0
4	DQ5	A	604	29/29	0.91	0.13	80,89,100,103	0
8	P6G	B	609	19/19	0.92	0.15	58,80,91,92	0
5	CL	A	608	1/1	0.96	0.05	67,67,67,67	0
5	CL	B	605	1/1	0.96	0.08	64,64,64,64	0
3	ELT	A	603	8/9	0.96	0.13	30,58,65,73	0
5	CL	B	608	1/1	0.97	0.06	48,48,48,48	0
5	CL	A	606	1/1	0.97	0.17	65,65,65,65	0
3	ELT	B	603	8/9	0.98	0.09	33,54,60,67	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.

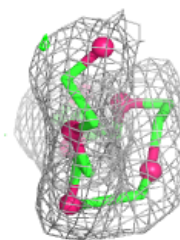
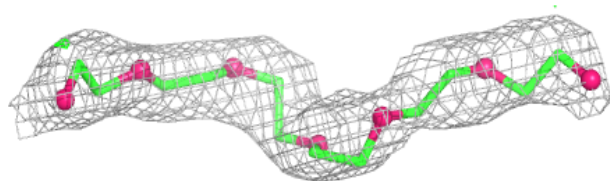
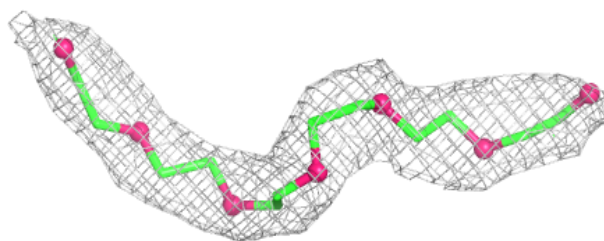
Electron density around DQ5 A 604:

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



Electron density around P6G B 609:

$2mF_o - DF_c$ (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.