



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:38 AM BST

PDB ID : 6G4P  
Title : Non-aged form of Torpedo californica acetylcholinesterase inhibited by tabun analog NEDPA bound to uncharged reactivator 2  
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 : 2.83 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

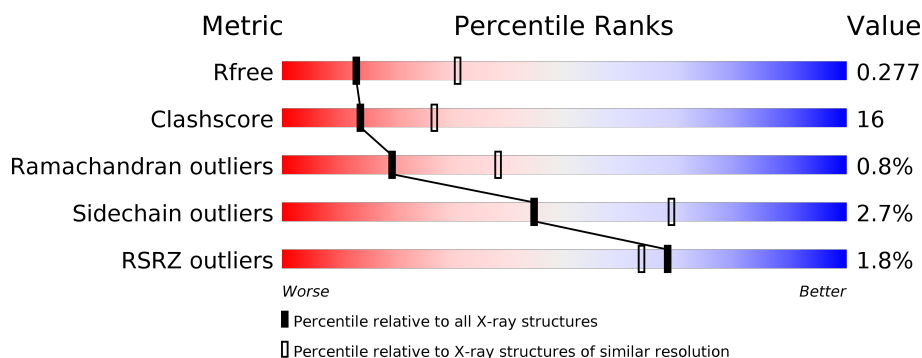
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 71% 27% ..
1	B	537	 3% 65% 32% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	606	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8716 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.

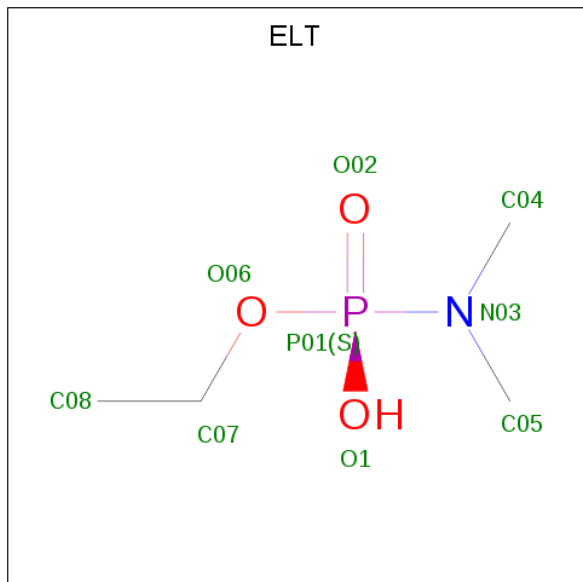
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4244	2721	720	781	22			
1	B	532	Total	C	N	O	S	0	1	0
			4252	2726	723	781	22			

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



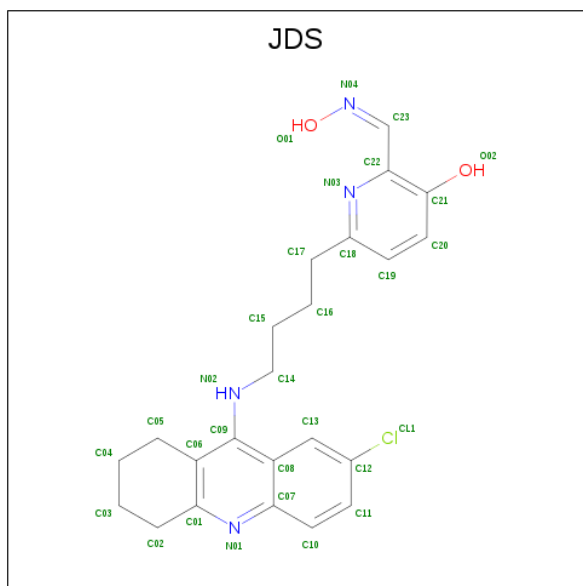
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ethoxy- {N}, {N}-dimethyl-phosphonamidic acid (three-letter code: 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 6-[4-[(7-chloranyl-1,2,3,4-tetrahydroacridin-9-yl)amino]butyl]-2-[( {Z})-hydrox yiminomethyl]pyridin-3-ol (three-letter code: JDS) (formula:  $C_{23}H_{25}ClN_4O_2$ ).

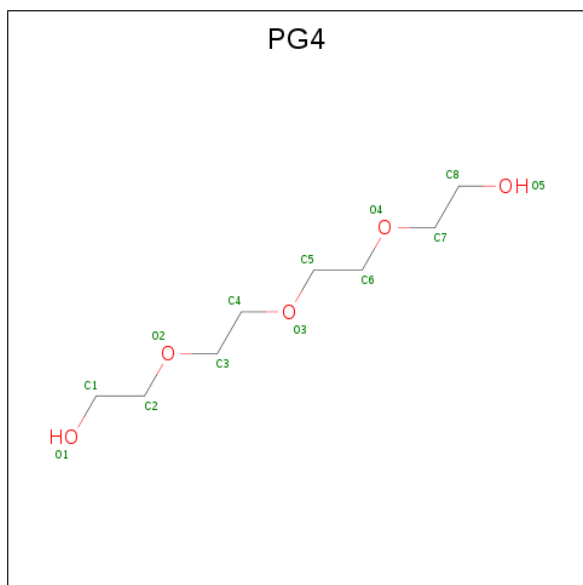


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	23	1	4	2		
4	B	1	Total	C	Cl	N	O	0	0
			30	23	1	4	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	30	Total	O	0	0
			30	30		

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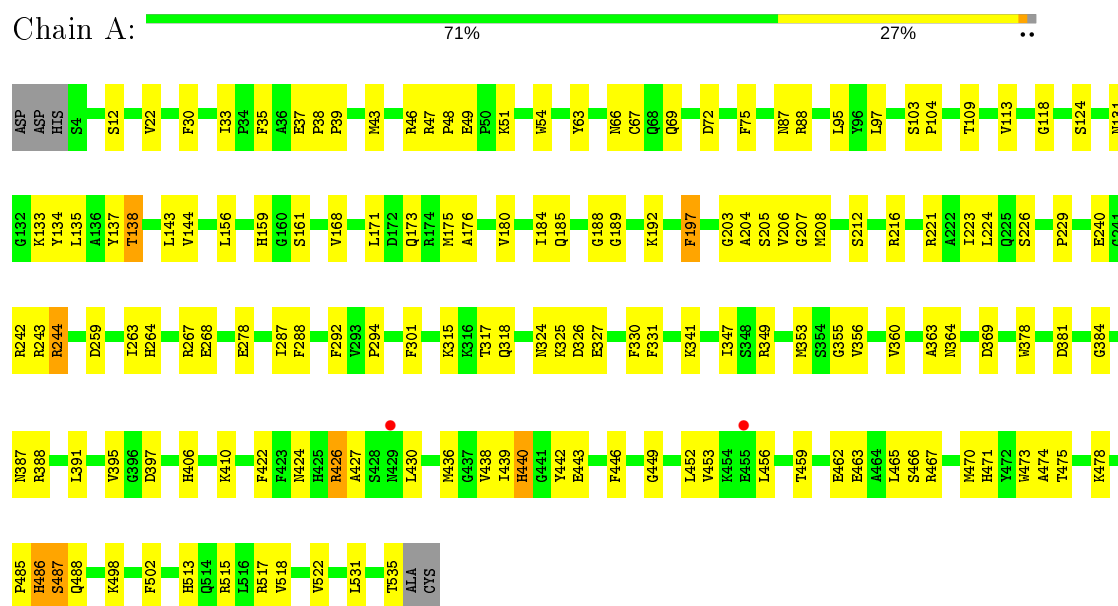
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	24	Total	O	0	0
			24	24		

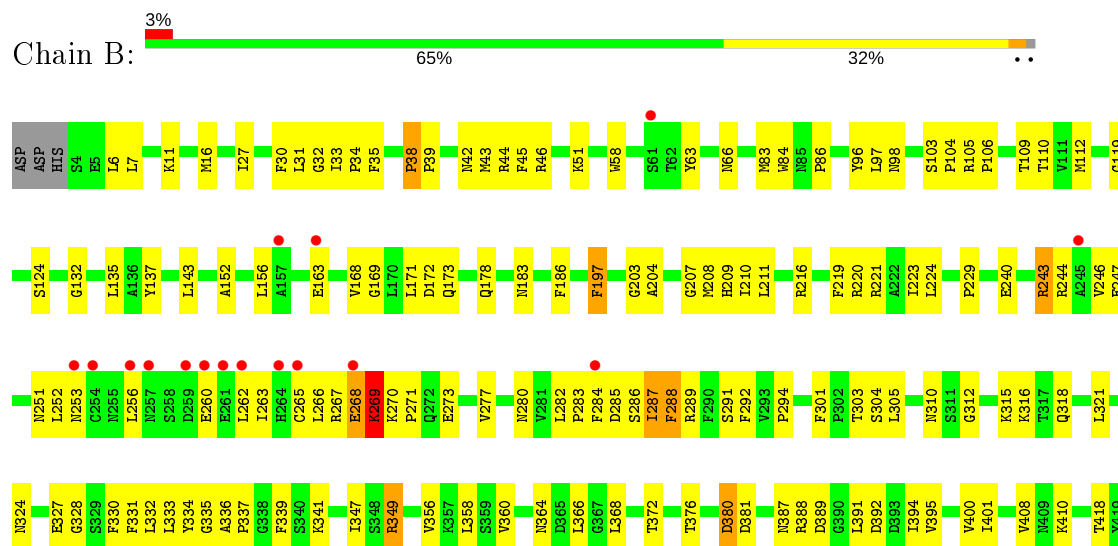
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	91.51Å 106.56Å 150.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.92 – 2.83 46.04 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.92-2.83) 98.7 (46.04-2.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.201 , 0.277 0.201 , 0.277	Depositor DCC
$R_{free}$ test set	1682 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 36.39 % 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 5.0317e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: PG4, ELT, NAG, JDS, 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	0.58	4/4367 (0.1%)	0.68	3/5929 (0.1%)
1	B	0.54	2/4378 (0.0%)	0.69	2/5943 (0.0%)
All	All	0.56	6/8745 (0.1%)	0.68	5/11872 (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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	ARG	NE-CZ	-8.92	1.21	1.33
1	A	426	ARG	CZ-NH1	-8.80	1.21	1.33
1	A	426	ARG	CZ-NH2	-7.69	1.23	1.33
1	A	426	ARG	CD-NE	-7.38	1.33	1.46
1	B	518	VAL	CB-CG1	-5.14	1.42	1.52
1	B	38	PRO	C-N	5.04	1.43	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	LYS	CD-CE-NZ	7.05	127.91	111.70
1	B	243	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	72	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	244	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	72	ASP	CB-CG-OD1	-5.38	113.46	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	268	GLU	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	4244	0	4095	104	0
1	B	4252	0	4108	168	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
5	A	3	0	0	0	0
5	B	5	0	0	2	0
6	A	13	0	18	1	0
6	B	13	0	18	3	0
7	A	30	0	0	1	0
7	B	24	0	0	2	0
All	All	8716	0	8291	268	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 16.

All (268) 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:269:LYS:HE2	1:B:269:LYS:H	1.20	1.02
1:B:266:LEU:CA	1:B:269:LYS:HE3	1.92	1.00
1:A:397:ASP:OD2	1:A:517:ARG:NH1	1.95	0.99
1:B:349:ARG:NH2	1:B:387:ASN:OD1	1.94	0.99
1:B:266:LEU:C	1:B:269:LYS:HE3	1.83	0.97
1:B:266:LEU:HA	1:B:269:LYS:HE3	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLU:H	1:B:269:LYS:HZ3	1.14	0.93
1:B:451:PRO:O	1:B:454:LYS:NZ	2.03	0.92
1:B:478:LYS:NZ	5:B:606:CL:CL	2.40	0.90
1:B:267:ARG:H	1:B:269:LYS:HZ1	1.17	0.90
1:B:349:ARG:NE	1:B:381:ASP:O	2.06	0.89
1:B:216:ARG:HG2	1:B:315:LYS:HB2	1.58	0.86
1:B:269:LYS:CE	1:B:269:LYS:H	1.92	0.82
1:A:369:ASP:OD1	1:B:530:LYS:NZ	2.15	0.79
1:B:267:ARG:N	1:B:269:LYS:HZ1	1.79	0.79
1:B:105:ARG:NH1	1:B:186:PHE:O	2.17	0.77
1:B:269:LYS:HE2	1:B:269:LYS:N	1.98	0.77
1:B:310:ASN:OD1	1:B:410:LYS:NZ	2.20	0.74
1:B:312:GLY:O	1:B:316:LYS:NZ	2.20	0.74
1:B:328:GLY:HA3	1:B:395:VAL:HG23	1.70	0.74
1:B:282:LEU:HD21	1:B:291:SER:HA	1.71	0.71
1:B:516:LEU:O	7:B:701:HOH:O	2.07	0.71
1:B:66:ASN:HD22	1:B:86:PRO:HB3	1.55	0.71
1:B:388[A]:ARG:NH2	1:B:389:ASP:OD1	2.24	0.71
1:B:265:CYS:O	1:B:269:LYS:NZ	2.23	0.70
1:A:159:HIS:O	1:A:242:ARG:NH1	2.24	0.70
1:A:135:LEU:HD13	1:A:470:MET:HG2	1.71	0.69
1:A:364:ASN:HD21	1:A:535:THR:HG23	1.58	0.68
1:B:267:ARG:N	1:B:269:LYS:NZ	2.41	0.68
1:B:252:LEU:HD21	1:B:277:VAL:HG11	1.75	0.68
1:B:211:LEU:HD13	1:B:305:LEU:HD22	1.76	0.66
1:B:132:GLY:HA3	1:B:143:LEU:HD23	1.78	0.66
1:B:324:ASN:HD22	1:B:440:HIS:HA	1.59	0.66
1:B:152:ALA:HA	1:B:292:PHE:HD1	1.59	0.66
1:B:34:PRO:HB2	1:B:51:LYS:HD3	1.76	0.66
1:A:67:CYS:O	1:A:69:GLN:HG3	1.95	0.66
1:B:143:LEU:HD21	1:B:448:PHE:HE2	1.59	0.66
1:B:266:LEU:HA	1:B:269:LYS:CE	2.23	0.65
1:A:378:TRP:H	1:B:519:GLN:HE22	1.45	0.65
1:B:391:LEU:HA	1:B:394:ILE:HD12	1.78	0.65
1:B:372:THR:O	1:B:376:THR:OG1	2.13	0.64
1:A:427:ALA:HB3	1:A:430:LEU:HD13	1.79	0.63
1:B:287:ILE:HG21	1:B:358:LEU:HB3	1.79	0.63
1:B:43:MET:HA	1:B:46:ARG:HD3	1.80	0.63
1:B:163:GLU:HB3	1:B:267:ARG:NH2	2.13	0.62
1:B:253:ASN:ND2	1:B:253:ASN:O	2.33	0.62
1:A:30:PHE:HB3	1:A:33:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.81	0.61
1:B:321:LEU:HD11	1:B:408:VAL:HG22	1.81	0.61
1:A:325:LYS:HG3	1:A:422:PHE:HZ	1.66	0.61
1:B:204:ALA:O	1:B:208:MET:HG3	2.01	0.60
1:A:134:TYR:O	1:A:138:THR:OG1	2.19	0.60
1:B:286:SER:OG	1:B:287:ILE:N	2.32	0.60
1:A:204:ALA:O	1:A:208:MET:HG3	2.01	0.60
1:A:349:ARG:HD3	1:A:381:ASP:O	2.02	0.60
1:A:168:VAL:HA	1:A:171:LEU:HD12	1.82	0.60
1:A:347:ILE:HG12	1:A:388:ARG:HB2	1.82	0.60
1:B:34:PRO:HB3	1:B:96:TYR:CE1	2.38	0.59
1:B:251:ASN:O	1:B:252:LEU:HD23	2.03	0.59
1:B:211:LEU:O	1:B:216:ARG:NH1	2.36	0.58
1:B:251:ASN:OD1	1:B:280:ASN:ND2	2.35	0.58
1:B:42:ASN:O	1:B:267:ARG:NH1	2.36	0.58
1:B:332:LEU:HD11	1:B:392:ASP:HA	1.85	0.58
1:B:266:LEU:C	1:B:269:LYS:CE	2.64	0.58
1:B:268:GLU:H	1:B:269:LYS:NZ	1.93	0.58
1:B:400:VAL:HG23	1:B:401:ILE:N	2.18	0.58
1:B:220:ARG:HG3	1:B:221:ARG:HG2	1.85	0.58
1:B:263:ILE:HG21	1:B:267:ARG:HH21	1.69	0.58
1:A:474:ALA:O	1:A:478:LYS:HG3	2.04	0.57
1:B:243:ARG:O	1:B:246:VAL:HG12	2.05	0.57
1:A:22:VAL:HG22	1:A:133:LYS:HD2	1.86	0.57
1:A:430:LEU:HD11	1:A:442:TYR:CD2	2.39	0.57
1:A:463:GLU:O	1:A:467:ARG:HG3	2.05	0.57
1:B:268:GLU:N	1:B:269:LYS:HZ3	1.95	0.57
1:B:321:LEU:O	1:B:420:LEU:HA	2.05	0.57
1:B:332:LEU:HD13	1:B:339:PHE:CZ	2.40	0.57
1:B:197:PHE:HB2	1:B:223:ILE:HB	1.87	0.56
1:B:246:VAL:CG2	1:B:256:LEU:HD23	2.35	0.56
1:B:388[A]:ARG:HG3	1:B:389:ASP:N	2.20	0.56
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.88	0.56
1:B:103:SER:HA	1:B:104:PRO:C	2.25	0.56
1:B:364:ASN:O	1:B:368:LEU:HG	2.06	0.56
1:A:39:PRO:HG3	1:A:95:LEU:CD1	2.36	0.56
1:B:45:PHE:CE1	1:B:156:LEU:HD13	2.41	0.56
1:B:44:ARG:HG2	1:B:45:PHE:CD2	2.40	0.56
1:B:163:GLU:HB3	1:B:267:ARG:HH22	1.70	0.55
1:A:88:ARG:NH1	7:A:701:HOH:O	2.16	0.55
1:A:259:ASP:O	1:A:263:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:CYS:C	1:B:269:LYS:NZ	2.60	0.55
1:B:266:LEU:CA	1:B:269:LYS:CE	2.76	0.55
1:B:463:GLU:O	1:B:467:ARG:HG3	2.08	0.54
1:A:353:MET:HA	1:A:356:VAL:HG12	1.89	0.54
1:A:518:VAL:O	1:A:522:VAL:HG23	2.07	0.54
1:B:388[B]:ARG:HG3	1:B:389:ASP:N	2.23	0.54
1:A:378:TRP:H	1:B:519:GLN:NE2	2.05	0.54
1:A:87:ASN:O	1:A:88:ARG:HD2	2.07	0.54
1:B:440:HIS:CE1	6:B:610:PG4:H71	2.43	0.53
1:A:131:ASN:HD21	1:A:133:LYS:HE2	1.73	0.53
1:B:119:GLY:N	3:B:603:ELT:O02	2.42	0.53
1:B:433:PRO:HD2	1:B:436:MET:SD	2.49	0.53
1:B:263:ILE:CG2	1:B:267:ARG:HE	2.22	0.53
1:B:515:ARG:HB3	1:B:518:VAL:CG1	2.39	0.53
1:B:267:ARG:N	1:B:269:LYS:CE	2.72	0.53
1:A:197:PHE:CB	1:A:223:ILE:HB	2.39	0.52
1:A:212:SER:O	1:A:216:ARG:HG3	2.09	0.52
1:B:11:LYS:H	1:B:183:ASN:ND2	2.06	0.52
1:A:206:VAL:CG2	1:A:224:LEU:HG	2.40	0.52
1:A:331:PHE:CE2	6:A:608:PG4:H21	2.44	0.52
1:B:152:ALA:HA	1:B:292:PHE:CD1	2.43	0.52
1:A:424:ASN:HA	1:A:438:VAL:HG21	1.91	0.52
1:B:207:GLY:O	1:B:210:ILE:HB	2.10	0.52
1:B:331:PHE:CD1	1:B:331:PHE:N	2.77	0.52
1:A:531:LEU:HG	1:B:366:LEU:HD21	1.92	0.52
1:A:203:GLY:O	1:A:206:VAL:HG22	2.10	0.51
1:B:287:ILE:N	7:B:705:HOH:O	2.42	0.51
1:B:265:CYS:C	1:B:269:LYS:HZ2	2.14	0.51
1:A:37:GLU:HG2	1:A:51:LYS:HA	1.93	0.51
1:B:221:ARG:NH2	1:B:478:LYS:O	2.43	0.51
1:A:531:LEU:O	1:A:535:THR:HG22	2.11	0.51
1:B:408:VAL:HG13	1:B:418:THR:HG21	1.93	0.51
1:A:240:GLU:O	1:A:244:ARG:HG3	2.10	0.50
1:A:208:MET:HG2	1:A:229:PRO:HB3	1.94	0.50
1:A:446:PHE:CE2	1:A:465:LEU:HD23	2.46	0.50
1:B:208:MET:HE1	1:B:294:PRO:HG2	1.94	0.50
1:A:221:ARG:NH1	1:A:318:GLN:OE1	2.42	0.50
1:A:173:GLN:HE22	1:A:205:SER:HB3	1.75	0.50
1:B:270:LYS:HB2	1:B:271:PRO:HD3	1.92	0.50
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.93	0.50
1:B:347:ILE:HD12	1:B:388[A]:ARG:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:O	1:B:284:PHE:N	2.39	0.49
1:B:341:LYS:O	1:B:433:PRO:HG3	2.12	0.49
1:A:263:ILE:O	1:A:267:ARG:HG3	2.12	0.49
1:B:6:LEU:O	1:B:16:MET:HA	2.13	0.49
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.93	0.49
1:B:334:TYR:CZ	6:B:610:PG4:H32	2.47	0.49
1:A:453:VAL:HG23	1:A:456:LEU:HG	1.95	0.49
1:A:360:VAL:HG12	1:A:363:ALA:HB2	1.95	0.49
1:A:406:HIS:CE1	1:A:410:LYS:HE3	2.48	0.49
1:A:208:MET:HB3	1:A:301:PHE:CE1	2.47	0.49
1:A:206:VAL:HG23	1:A:224:LEU:HG	1.94	0.49
1:A:426:ARG:HG3	1:A:426:ARG:HH21	1.77	0.49
1:B:243:ARG:HD2	1:B:247:GLU:OE1	2.12	0.49
1:B:265:CYS:O	1:B:269:LYS:CE	2.61	0.49
1:B:446:PHE:O	1:B:466:SER:OG	2.25	0.48
1:A:439:ILE:HB	1:A:442:TYR:CD1	2.48	0.48
1:B:282:LEU:CD2	1:B:291:SER:HA	2.43	0.48
1:B:364:ASN:N	1:B:364:ASN:OD1	2.45	0.48
1:A:287:ILE:HD11	1:A:395:VAL:HG21	1.95	0.48
1:A:12:SER:HB3	1:A:54:TRP:CZ3	2.48	0.48
1:A:35:PHE:CD2	1:A:97:LEU:HD23	2.48	0.48
1:B:453:VAL:HG12	1:B:455:GLU:HG2	1.94	0.48
1:A:422:PHE:CE1	1:A:424:ASN:HB3	2.49	0.48
1:B:203:GLY:O	1:B:224:LEU:HD23	2.14	0.48
1:B:168:VAL:HA	1:B:171:LEU:HD12	1.96	0.48
1:B:347:ILE:HG22	1:B:387:ASN:HB3	1.94	0.48
1:B:106:PRO:HB2	1:B:109:THR:OG1	2.14	0.48
1:B:240:GLU:CD	1:B:243:ARG:HH21	2.17	0.48
1:B:518:VAL:O	1:B:522:VAL:HG23	2.14	0.48
1:B:135:LEU:HD13	1:B:470:MET:HG2	1.96	0.47
1:B:240:GLU:OE2	1:B:243:ARG:NH2	2.46	0.47
1:B:208:MET:HB3	1:B:301:PHE:HE1	1.78	0.47
1:B:510:MET:HG2	1:B:511:LYS:N	2.30	0.47
1:A:208:MET:HE3	1:A:294:PRO:HG2	1.97	0.47
1:B:526:GLN:O	1:B:530:LYS:HE2	2.14	0.47
1:B:243:ARG:HD2	1:B:247:GLU:CD	2.35	0.47
1:A:498:LYS:HD3	1:A:498:LYS:HA	1.71	0.47
1:B:30:PHE:HB3	1:B:33:ILE:HD11	1.97	0.47
1:B:84:TRP:CE3	6:B:610:PG4:H82	2.50	0.47
1:B:35:PHE:CD2	1:B:97:LEU:HD23	2.50	0.47
1:A:226:SER:OG	1:A:327:GLU:OE1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:HE1	1:A:49:GLU:CG	2.45	0.46
1:B:347:ILE:HD12	1:B:388[A]:ARG:CB	2.45	0.46
1:B:516:LEU:HD23	1:B:517:ARG:HB2	1.98	0.46
1:A:471:HIS:CD2	1:A:475:THR:HG23	2.51	0.46
1:B:267:ARG:H	1:B:269:LYS:NZ	1.96	0.46
1:B:349:ARG:CD	1:B:381:ASP:HB2	2.46	0.46
1:B:244:ARG:NH1	1:B:291:SER:O	2.49	0.46
1:B:430:LEU:HA	1:B:430:LEU:HD12	1.81	0.46
1:A:459:THR:HB	1:A:462:GLU:OE1	2.16	0.46
1:A:268:GLU:CD	1:A:268:GLU:N	2.70	0.45
1:B:303:THR:HG22	1:B:304:SER:N	2.31	0.45
1:B:388[A]:ARG:CZ	1:B:435:TRP:HB2	2.47	0.45
1:B:356:VAL:HG12	1:B:394:ILE:HD13	1.98	0.45
1:A:452:LEU:HD21	1:A:467:ARG:HG2	1.99	0.45
1:A:176:ALA:O	1:A:180:VAL:HG23	2.16	0.45
1:B:208:MET:HG2	1:B:229:PRO:HB3	1.98	0.45
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.52	0.45
1:B:262:LEU:O	1:B:266:LEU:HG	2.17	0.45
1:B:27:ILE:HG21	1:B:137:TYR:HB2	1.99	0.45
1:B:291:SER:OG	1:B:292:PHE:N	2.50	0.45
1:B:152:ALA:CA	1:B:292:PHE:HD1	2.29	0.45
1:A:315:LYS:HG2	1:A:317:THR:HG22	1.98	0.44
1:B:288:PHE:O	1:B:289:ARG:HD3	2.16	0.44
1:B:324:ASN:N	1:B:327:GLU:OE2	2.46	0.44
1:B:32:GLY:H	1:B:98:ASN:ND2	2.16	0.44
1:A:278:GLU:HG3	1:A:292:PHE:HE2	1.82	0.44
1:A:268:GLU:N	1:A:268:GLU:OE2	2.50	0.44
1:B:368:LEU:O	1:B:372:THR:OG1	2.26	0.44
1:A:103:SER:HA	1:A:104:PRO:C	2.37	0.44
1:B:38:PRO:HA	1:B:39:PRO:HD3	1.88	0.44
1:B:34:PRO:HG3	1:B:58:TRP:CH2	2.52	0.44
1:B:246:VAL:HG22	1:B:256:LEU:HD23	2.00	0.44
1:A:113:VAL:HG22	1:A:144:VAL:HB	2.00	0.44
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.71	0.44
1:A:66:ASN:ND2	1:A:124:SER:HB3	2.33	0.44
1:A:287:ILE:HD11	1:A:395:VAL:CG2	2.48	0.44
1:B:109:THR:HG22	1:B:110:THR:N	2.33	0.44
1:B:347:ILE:HD12	1:B:388[B]:ARG:HB3	1.98	0.44
1:B:173:GLN:NE2	1:B:209:HIS:NE2	2.66	0.43
1:B:219:PHE:O	1:B:315:LYS:HE2	2.18	0.43
1:B:246:VAL:HG23	1:B:256:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HG3	1:A:95:LEU:HD12	1.99	0.43
1:B:208:MET:HB3	1:B:301:PHE:CE1	2.53	0.43
1:A:46:ARG:HG3	1:A:47:ARG:N	2.34	0.43
1:A:137:TYR:CD1	1:A:138:THR:HG23	2.54	0.43
1:A:349:ARG:HH11	1:A:387:ASN:ND2	2.17	0.43
1:A:426:ARG:HG3	1:A:426:ARG:NH2	2.34	0.43
1:B:262:LEU:O	1:B:262:LEU:HD12	2.19	0.43
1:B:178:GLN:HG3	1:B:178:GLN:O	2.19	0.42
1:B:270:LYS:HG2	1:B:273:GLU:OE2	2.19	0.42
1:B:32:GLY:H	1:B:98:ASN:HD22	1.65	0.42
1:A:48:PRO:HB2	1:A:175:MET:HE3	2.01	0.42
1:B:356:VAL:O	1:B:360:VAL:HG22	2.20	0.42
1:B:42:ASN:OD1	1:B:42:ASN:N	2.51	0.42
1:A:208:MET:CE	1:A:294:PRO:HG2	2.50	0.42
1:B:197:PHE:CB	1:B:223:ILE:HB	2.50	0.42
1:B:263:ILE:HG22	1:B:267:ARG:HE	1.84	0.42
1:A:185:GLN:HA	1:A:189:GLY:O	2.18	0.42
1:B:112:MET:HB2	1:B:143:LEU:HD12	2.00	0.42
1:B:207:GLY:HA3	1:B:229:PRO:HD3	2.01	0.42
1:A:324:ASN:ND2	1:A:443:GLU:OE1	2.53	0.42
1:A:449:GLY:HA2	1:A:466:SER:OG	2.18	0.42
1:A:135:LEU:HA	1:A:470:MET:CE	2.49	0.42
1:B:270:LYS:HE3	1:B:270:LYS:HB2	1.66	0.42
1:B:336:ALA:HB1	1:B:337:PRO:HD2	2.02	0.42
1:B:388[B]:ARG:HG3	1:B:389:ASP:H	1.83	0.42
1:A:436:MET:HB3	1:A:439:ILE:CD1	2.49	0.42
1:A:453:VAL:CG2	1:A:456:LEU:HG	2.50	0.42
1:B:221:ARG:NH1	1:B:318:GLN:OE1	2.53	0.42
1:A:43:MET:HE1	1:A:49:GLU:HG2	2.02	0.41
1:A:264:HIS:O	1:A:268:GLU:OE2	2.38	0.41
1:B:270:LYS:O	1:B:273:GLU:HB2	2.20	0.41
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.55	0.41
1:A:137:TYR:HD1	1:A:138:THR:HG23	1.86	0.41
1:A:39:PRO:HG3	1:A:95:LEU:HD11	2.02	0.41
1:B:169:GLY:HA2	1:B:172:ASP:OD2	2.20	0.41
1:A:75:PHE:CE1	1:A:341:LYS:HD3	2.54	0.41
1:A:341:LYS:HZ2	1:A:341:LYS:HG2	1.77	0.41
1:A:43:MET:HE2	1:A:43:MET:HB3	1.79	0.41
1:B:431:VAL:H	1:B:431:VAL:HG22	1.61	0.41
1:A:135:LEU:HD23	1:A:143:LEU:HD22	2.02	0.41
1:B:287:ILE:HG13	1:B:287:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:HD23	1:B:334:TYR:CE1	2.56	0.41
1:A:325:LYS:HG3	1:A:422:PHE:CZ	2.51	0.41
1:A:325:LYS:NZ	1:A:326:ASP:OD2	2.53	0.41
1:A:486:HIS:ND1	1:A:488:GLN:HB2	2.36	0.41
1:B:324:ASN:OD1	1:B:423:PHE:HB3	2.20	0.41
1:B:484:GLU:O	1:B:487:SER:HB3	2.20	0.41
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.99	0.40
1:A:192:LYS:HE3	1:A:192:LYS:HB3	1.83	0.40
1:B:31:LEU:HD23	1:B:98:ASN:HB3	2.03	0.40
1:A:109:THR:HG22	1:A:188:GLY:O	2.22	0.40
1:A:440:HIS:ND1	1:A:440:HIS:O	2.54	0.40
1:B:260:GLU:N	1:B:260:GLU:OE2	2.52	0.40
1:B:280:ASN:N	1:B:280:ASN:OD1	2.51	0.40
1:B:471:HIS:CE1	5:B:606:CL:CL	3.11	0.40
1:A:485:PRO:O	1:A:487:SER:N	2.53	0.40
1:B:273:GLU:O	1:B:277:VAL:HG22	2.22	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	530/537 (99%)	491 (93%)	35 (7%)	4 (1%)	19	38
1	B	531/537 (99%)	490 (92%)	36 (7%)	5 (1%)	17	34
All	All	1061/1074 (99%)	981 (92%)	71 (7%)	9 (1%)	19	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	HIS
1	A	487	SER

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Mol	Chain	Res	Type
1	B	287	ILE
1	B	335	GLY
1	B	380	ASP
1	B	515	ARG
1	B	283	PRO
1	A	384	GLY
1	A	118	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	465/469 (99%)	455 (98%)	10 (2%)	52	75
1	B	466/469 (99%)	451 (97%)	15 (3%)	39	63
All	All	931/938 (99%)	906 (97%)	25 (3%)	44	69

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

Mol	Chain	Res	Type
1	A	63	TYR
1	A	138	THR
1	A	156	LEU
1	A	161	SER
1	A	197	PHE
1	A	243	ARG
1	A	288	PHE
1	A	330	PHE
1	A	440	HIS
1	A	473	TRP
1	B	7	LEU
1	B	63	TYR
1	B	83	MET
1	B	124	SER
1	B	197	PHE
1	B	269	LYS

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Mol	Chain	Res	Type
1	B	285	ASP
1	B	288	PHE
1	B	330	PHE
1	B	349	ARG
1	B	380	ASP
1	B	428	SER
1	B	483	ASN
1	B	486	HIS
1	B	517	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	173	GLN
1	A	387	ASN
1	A	471	HIS
1	B	66	ASN
1	B	98	ASN
1	B	131	ASN
1	B	162	GLN
1	B	173	GLN
1	B	183	ASN
1	B	440	HIS
1	B	519	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 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
4	JDS	A	604	-	33,33,33	1.82	11 (33%)	40,45,45	1.87	10 (25%)
3	ELT	B	603	1	4,7,8	1.63	2 (50%)	4,8,11	0.91	0
2	NAG	A	601	1	14,14,15	0.50	0	17,19,21	0.74	1 (5%)
2	NAG	A	602	1	14,14,15	0.72	1 (7%)	17,19,21	0.93	1 (5%)
6	PG4	A	608	-	12,12,12	0.65	0	11,11,11	0.90	0
2	NAG	B	602	1	14,14,15	0.84	1 (7%)	17,19,21	0.73	0
2	NAG	B	601	1	14,14,15	0.79	1 (7%)	17,19,21	0.75	1 (5%)
6	PG4	B	610	-	12,12,12	0.74	0	11,11,11	0.91	0
3	ELT	A	603	1	4,7,8	1.37	0	4,8,11	1.37	1 (25%)
4	JDS	B	604	-	33,33,33	1.27	2 (6%)	40,45,45	1.56	7 (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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JDS	A	604	-	-	5/11/18/18	0/4/4/4
3	ELT	B	603	1	-	0/1/7/10	-
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	PG4	A	608	-	-	6/10/10/10	-
2	NAG	B	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
6	PG4	B	610	-	-	5/10/10/10	-
3	ELT	A	603	1	-	0/1/7/10	-
4	JDS	B	604	-	-	5/11/18/18	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	JDS	C22-N03	3.70	1.39	1.35
4	B	604	JDS	C06-C01	3.62	1.45	1.40
4	A	604	JDS	C14-N02	3.52	1.53	1.45
4	A	604	JDS	C06-C01	3.40	1.45	1.40
4	B	604	JDS	O01-N04	-3.22	1.33	1.40
4	A	604	JDS	C23-N04	3.08	1.33	1.27
4	A	604	JDS	C17-C18	2.97	1.57	1.51
4	A	604	JDS	C18-N03	2.66	1.39	1.34
4	A	604	JDS	C22-C23	2.62	1.52	1.47
2	A	602	NAG	O5-C1	2.54	1.47	1.43
2	B	601	NAG	O5-C1	2.51	1.47	1.43
2	B	602	NAG	O5-C1	2.50	1.47	1.43
4	A	604	JDS	C09-N02	2.36	1.44	1.37
4	A	604	JDS	C12-CL1	-2.33	1.69	1.74
4	A	604	JDS	C15-C14	2.20	1.60	1.51
3	B	603	ELT	C04-N03	-2.18	1.42	1.45
4	A	604	JDS	C09-C06	2.17	1.42	1.38
3	B	603	ELT	C05-N03	2.01	1.49	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	JDS	C05-C06-C01	-4.95	116.45	121.08
4	A	604	JDS	O01-N04-C23	4.67	120.11	111.86
4	B	604	JDS	C05-C06-C01	-4.37	116.99	121.08
4	A	604	JDS	C06-C09-N02	4.14	127.13	119.54
2	A	602	NAG	C1-O5-C5	2.94	116.18	112.19
4	A	604	JDS	C17-C18-N03	2.91	120.29	115.95
4	A	604	JDS	C23-C22-N03	2.90	121.52	115.69
4	B	604	JDS	C17-C18-N03	2.72	120.00	115.95
4	B	604	JDS	O01-N04-C23	2.69	116.62	111.86
4	A	604	JDS	C08-C09-N02	-2.62	113.50	122.06
2	A	601	NAG	C1-O5-C5	2.57	115.67	112.19
4	B	604	JDS	C19-C20-C21	-2.53	117.90	120.50
4	A	604	JDS	C21-C22-C23	-2.39	118.01	121.55
4	B	604	JDS	C06-C09-N02	2.34	123.83	119.54
4	B	604	JDS	C15-C14-N02	2.30	117.67	111.49
4	A	604	JDS	C14-N02-C09	2.25	133.77	121.78
4	B	604	JDS	C06-C01-N01	-2.21	121.79	123.68
4	A	604	JDS	C16-C17-C18	2.16	119.90	113.11
4	A	604	JDS	C06-C01-N01	-2.10	121.89	123.68
2	B	601	NAG	C1-O5-C5	2.10	115.04	112.19

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	ELT	P01-N03-C05	-2.01	112.36	121.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	604	JDS	N02-C14-C15-C16
2	B	602	NAG	O5-C5-C6-O6
2	B	602	NAG	C4-C5-C6-O6
6	B	610	PG4	O2-C3-C4-O3
2	B	601	NAG	C4-C5-C6-O6
2	A	602	NAG	O5-C5-C6-O6
4	A	604	JDS	C15-C16-C17-C18
2	B	601	NAG	O5-C5-C6-O6
4	B	604	JDS	C08-C09-N02-C14
4	A	604	JDS	N02-C14-C15-C16
6	A	608	PG4	O4-C7-C8-O5
2	A	602	NAG	C4-C5-C6-O6
6	B	610	PG4	O3-C5-C6-O4
4	A	604	JDS	C15-C14-N02-C09
4	A	604	JDS	C06-C09-N02-C14
6	A	608	PG4	C5-C6-O4-C7
6	A	608	PG4	C4-C3-O2-C2
4	A	604	JDS	C14-C15-C16-C17
6	B	610	PG4	C4-C3-O2-C2
6	A	608	PG4	C3-C4-O3-C5
4	B	604	JDS	C16-C17-C18-C19
6	B	610	PG4	C5-C6-O4-C7
4	B	604	JDS	C16-C17-C18-N03
6	A	608	PG4	O3-C5-C6-O4
6	B	610	PG4	C1-C2-O2-C3
6	A	608	PG4	C1-C2-O2-C3
4	B	604	JDS	C15-C16-C17-C18

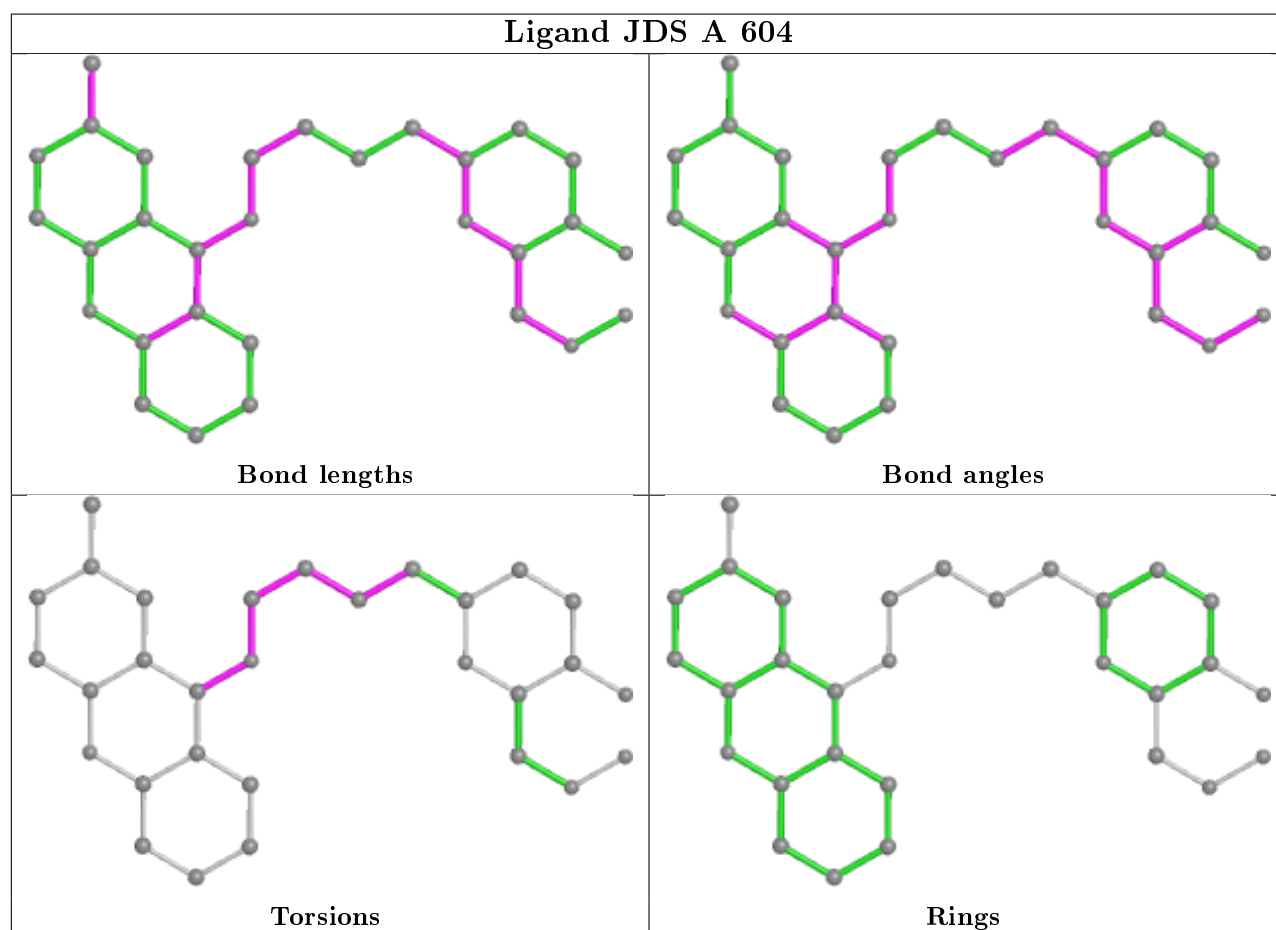
There are no ring outliers.

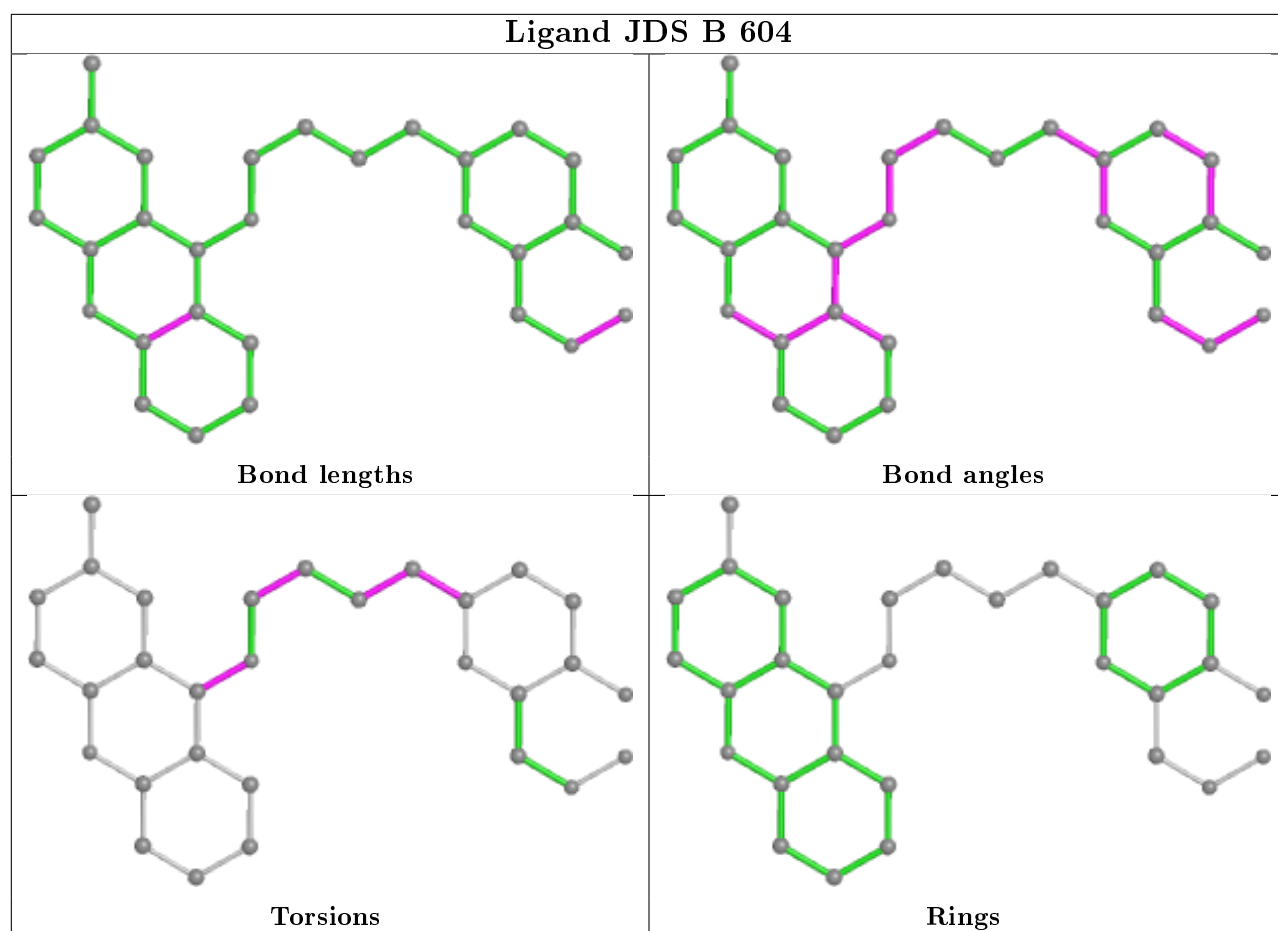
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	ELT	1	0
6	A	608	PG4	1	0
6	B	610	PG4	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	532/537 (99%)	-0.28	2 (0%) 92 91	25, 44, 76, 132	0
1	B	532/537 (99%)	-0.06	17 (3%) 47 41	27, 53, 95, 158	0
All	All	1064/1074 (99%)	-0.17	19 (1%) 68 63	25, 48, 86, 158	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	257	ASN	5.0
1	B	535	THR	3.4
1	B	265	CYS	3.1
1	B	261	GLU	3.1
1	A	429	ASN	3.1
1	B	256	LEU	3.0
1	B	163	GLU	2.8
1	B	253	ASN	2.8
1	A	455	GLU	2.8
1	B	245	ALA	2.8
1	B	254	CYS	2.8
1	B	268	GLU	2.7
1	B	262	LEU	2.7
1	B	157	ALA	2.7
1	B	61	SER	2.6
1	B	259	ASP	2.6
1	B	264	HIS	2.3
1	B	260	GLU	2.3
1	B	284	PHE	2.2

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

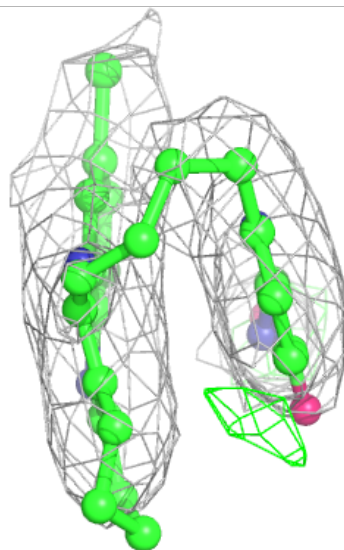
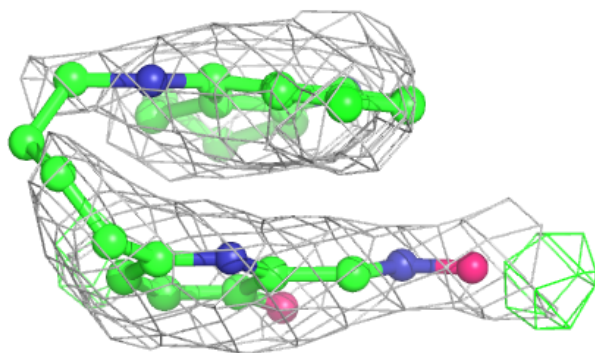
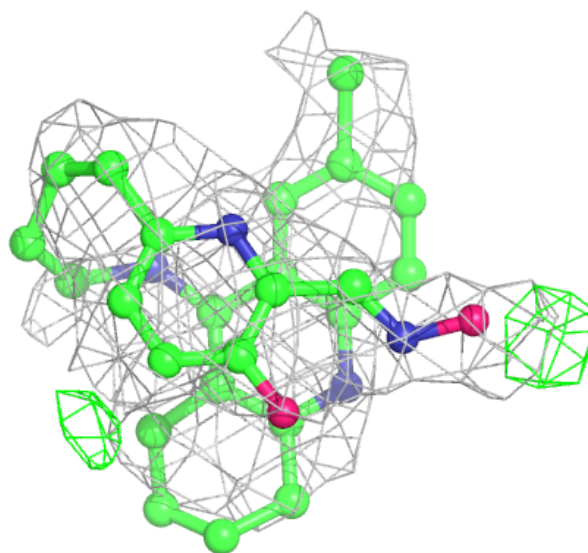
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	CL	B	605	1/1	0.76	0.20	60,60,60,60	0
5	CL	B	608	1/1	0.79	0.28	97,97,97,97	0
5	CL	B	606	1/1	0.79	0.28	114,114,114,114	0
2	NAG	B	602	14/15	0.83	0.20	41,70,88,90	0
5	CL	A	606	1/1	0.83	0.15	57,57,57,57	0
2	NAG	A	601	14/15	0.83	0.34	67,83,94,97	0
2	NAG	B	601	14/15	0.86	0.21	61,83,88,91	0
4	JDS	A	604	30/30	0.86	0.27	44,81,108,117	0
2	NAG	A	602	14/15	0.87	0.16	55,72,81,87	0
6	PG4	A	608	13/13	0.87	0.29	44,84,96,96	0
5	CL	B	609	1/1	0.89	0.09	90,90,90,90	0
5	CL	A	605	1/1	0.91	0.13	71,71,71,71	0
5	CL	B	607	1/1	0.92	0.07	69,69,69,69	0
5	CL	A	607	1/1	0.93	0.11	68,68,68,68	0
4	JDS	B	604	30/30	0.93	0.22	38,60,79,89	0
6	PG4	B	610	13/13	0.94	0.25	39,61,68,70	0
3	ELT	A	603	8/9	0.98	0.20	42,51,65,78	0
3	ELT	B	603	8/9	0.99	0.16	31,56,67,77	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.

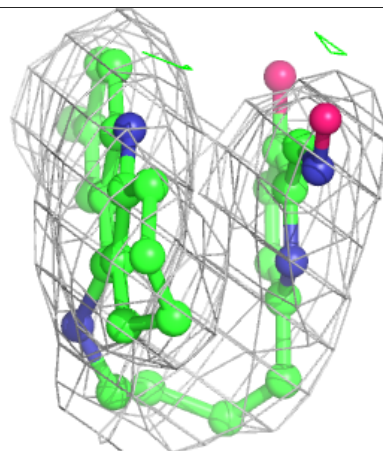
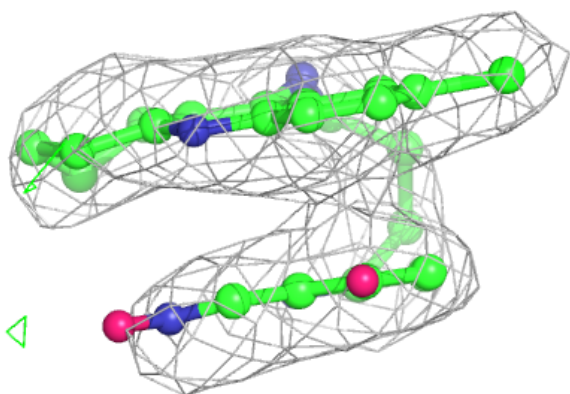
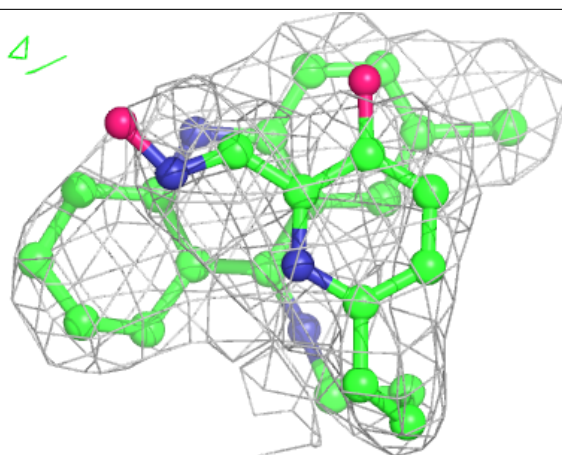
**Electron density around JDS A 604:**

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



**Electron density around JDS B 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 ⓘ

There are no such residues in this entry.