



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:07 PM UTC

PDB ID : 8AXP / pdb_00008axp
Title : Neisseria gonorrhoeae peptidyl-tRNA hydrolase complexed with an XChem hit.
Authors : Roe, S.M.; Fearon, D.
Deposited on : 2022-08-31
Resolution : 1.83 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

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

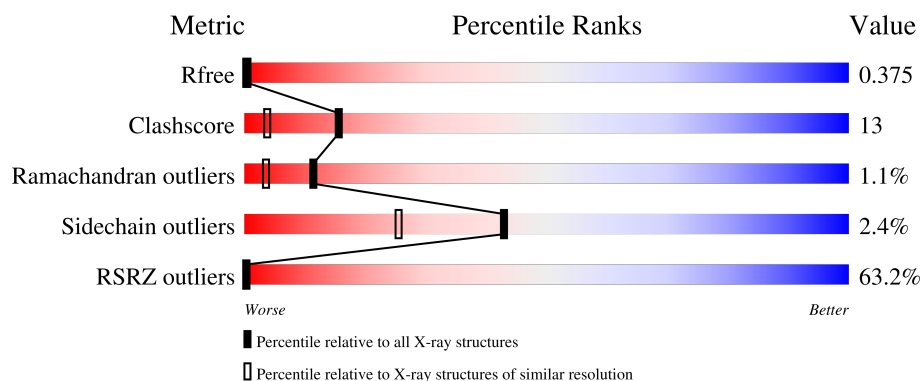
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	192	60% 70% 28% ..
1	B	192	65% 72% 24% ..

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
3	SO4	A	202	-	-	X	-

2 Entry composition [i](#)

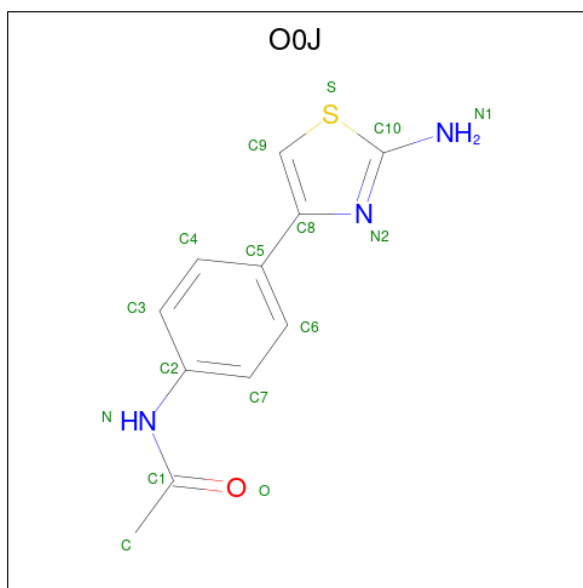
There are 4 unique types of molecules in this entry. The entry contains 3324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidyl-tRNA hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	189	Total	C	N	O	S	0	0	0
			1465	943	258	261	3			
1	A	191	Total	C	N	O	S	0	0	0
			1500	961	268	268	3			

- Molecule 2 is N-[4-(2-amino-1,3-thiazol-4-yl)phenyl]acetamide (CCD ID: O0J) (formula: C₁₁H₁₁N₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			16	11	3	1	1		
2	A	1	Total	C	N	O	S	0	0
			16	11	3	1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

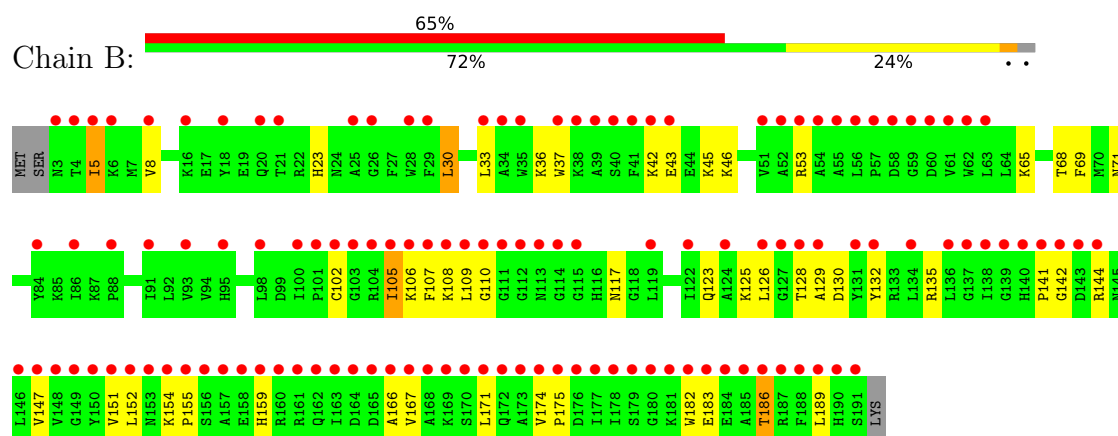
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	135	Total	O	0	0
			135	135		
4	A	157	Total	O	0	0
			157	157		

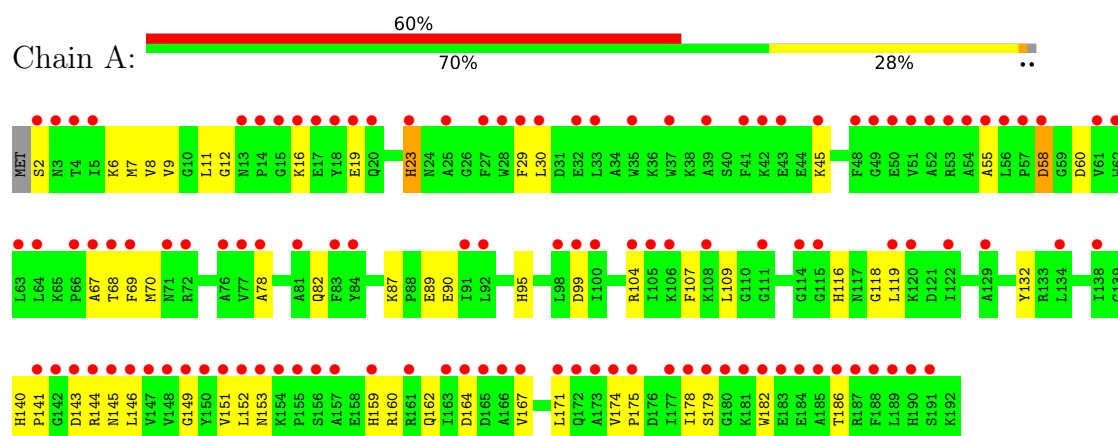
3 Residue-property plots [i](#)

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: Peptidyl-tRNA hydrolase



• Molecule 1: Peptidyl-tRNA hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.44Å 71.51Å 146.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.40 – 1.83 37.40 – 1.83	Depositor EDS
% Data completeness (in resolution range)	90.9 (37.40-1.83) 92.0 (37.40-1.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5..8.0349, PHENIX 1.20_4459	Depositor
R, R_{free}	0.335 , 0.364 0.346 , 0.375	Depositor DCC
R_{free} test set	1947 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3324	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: O0J, SO4

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	0.26	0/1537	0.51	0/2075
1	B	0.25	0/1502	0.52	0/2032
All	All	0.26	0/3039	0.52	0/4107

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1500	0	1486	41	0
1	B	1465	0	1435	36	0
2	A	16	0	0	0	0
2	B	16	0	0	1	0
3	A	15	0	0	2	0
3	B	20	0	0	1	0
4	A	157	0	0	12	1
4	B	135	0	0	14	1
All	All	3324	0	2921	80	1

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 13.

All (80) 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:7:MET:SD	4:A:394:HOH:O	2.23	0.95
1:A:11:LEU:HB3	1:A:70:MET:HE1	1.57	0.87
1:A:7:MET:HE2	1:A:9:VAL:HG22	1.65	0.77
1:B:65:LYS:NZ	4:B:304:HOH:O	2.17	0.76
1:A:70:MET:HE2	1:A:118:GLY:HA3	1.68	0.75
1:B:105:ILE:HD11	1:B:166:ALA:HA	1.71	0.72
1:A:89:GLU:OE1	4:A:301:HOH:O	2.06	0.72
3:A:202:SO4:O2	4:A:302:HOH:O	2.10	0.69
1:B:46:LYS:NZ	4:B:308:HOH:O	2.23	0.69
1:A:12:GLY:O	4:A:303:HOH:O	2.13	0.67
1:B:126:LEU:O	4:B:301:HOH:O	2.13	0.66
1:B:154:LYS:N	1:B:154:LYS:HD3	2.11	0.64
1:A:144:ARG:NH1	4:A:313:HOH:O	2.31	0.64
1:B:154:LYS:HD3	1:B:154:LYS:H	1.62	0.62
1:A:2:SER:N	1:A:58:ASP:O	2.32	0.62
1:B:102:CYS:SG	1:B:159:HIS:HB3	2.39	0.61
1:B:142:GLY:O	4:B:302:HOH:O	2.17	0.59
1:B:108:LYS:HD3	1:B:135:ARG:HE	1.66	0.59
1:B:71:ASN:OD1	4:B:303:HOH:O	2.17	0.58
1:A:167:VAL:O	1:A:171:LEU:HD13	2.03	0.58
1:A:174:VAL:HG13	1:A:178:ILE:CD1	2.35	0.57
2:B:201:O0J:N1	4:B:314:HOH:O	2.33	0.57
1:A:58:ASP:OD2	4:A:305:HOH:O	2.18	0.56
1:A:140:HIS:ND1	1:A:141:PRO:O	2.39	0.56
1:B:110:GLY:HA3	4:B:305:HOH:O	2.06	0.54
1:A:87:LYS:NZ	4:A:310:HOH:O	2.25	0.54
1:A:174:VAL:HG13	1:A:178:ILE:HD13	1.88	0.54
1:B:174:VAL:HG23	1:B:175:PRO:HD3	1.89	0.54
1:A:11:LEU:HD12	1:A:95:HIS:HB3	1.90	0.54
1:A:45:LYS:O	4:A:306:HOH:O	2.18	0.53
1:B:45:LYS:NZ	4:B:317:HOH:O	2.42	0.53
1:B:182:TRP:O	1:B:186:THR:HB	2.09	0.53
1:A:99:ASP:O	4:A:307:HOH:O	2.19	0.52
1:A:68:THR:O	1:A:69:PHE:HB2	2.09	0.51
1:B:5:ILE:HD12	4:B:347:HOH:O	2.09	0.51
1:A:182:TRP:O	1:A:186:THR:HG23	2.12	0.50
1:B:183:GLU:OE1	1:B:183:GLU:N	2.42	0.50
1:B:8:VAL:HG12	1:B:30:LEU:HD11	1.94	0.49
1:B:135:ARG:NH2	3:B:202:SO4:O1	2.45	0.49
1:B:53:ARG:NH1	4:B:312:HOH:O	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HB2	4:A:341:HOH:O	2.12	0.49
1:B:106:LYS:HG3	1:B:107:PHE:N	2.28	0.49
1:B:33:LEU:HD11	1:B:37:TRP:CZ3	2.47	0.49
1:A:159:HIS:HA	1:A:162:GLN:OE1	2.13	0.48
3:A:202:SO4:O2	4:A:309:HOH:O	2.20	0.48
1:B:42:LYS:HD3	1:B:43:GLU:O	2.14	0.47
1:A:145:ASN:ND2	4:A:324:HOH:O	2.48	0.47
1:B:36:LYS:HE2	1:B:174:VAL:HG21	1.97	0.47
1:B:106:LYS:HG3	1:B:107:PHE:H	1.79	0.47
1:B:130:ASP:OD1	4:B:305:HOH:O	2.21	0.47
1:A:95:HIS:CE1	1:A:119:LEU:HD11	2.50	0.46
1:A:175:PRO:O	1:A:179:SER:OG	2.31	0.46
1:B:117:ASN:OD1	1:B:117:ASN:N	2.47	0.46
1:B:125:LYS:O	4:B:307:HOH:O	2.21	0.45
1:A:70:MET:CE	1:A:118:GLY:HA3	2.43	0.45
1:A:109:LEU:HB2	1:A:132:TYR:CE1	2.52	0.45
1:B:167:VAL:O	1:B:171:LEU:HG	2.18	0.44
1:B:171:LEU:O	1:B:174:VAL:HG22	2.17	0.44
4:B:410:HOH:O	1:A:104:ARG:HD3	2.16	0.44
1:A:151:VAL:HG23	1:A:152:LEU:HD13	2.00	0.44
1:A:55:ALA:HA	1:A:60:ASP:OD2	2.18	0.44
1:B:123:GLN:NE2	1:B:129:ALA:HB2	2.33	0.44
1:A:143:ASP:OD1	1:A:144:ARG:N	2.50	0.43
1:A:149:GLY:O	1:A:153:ASN:ND2	2.32	0.43
1:B:144:ARG:HA	1:B:147:VAL:HG23	2.00	0.43
1:B:189:LEU:O	4:B:306:HOH:O	2.21	0.43
1:A:6:LYS:HE3	1:A:90:GLU:OE2	2.18	0.43
1:B:105:ILE:HD11	1:B:166:ALA:CA	2.45	0.42
1:B:109:LEU:HD22	1:B:132:TYR:CZ	2.54	0.42
1:A:55:ALA:HA	1:A:60:ASP:CG	2.44	0.42
1:A:78:ALA:O	1:A:82:GLN:HG2	2.19	0.42
1:A:16:LYS:HA	1:A:19:GLU:HB2	2.00	0.42
1:A:23:HIS:HB2	1:A:151:VAL:O	2.20	0.42
1:A:29:PHE:HD2	1:A:30:LEU:HD12	1.84	0.42
1:B:68:THR:O	1:B:69:PHE:HB2	2.19	0.41
1:A:107:PHE:HD2	1:A:186:THR:HG22	1.85	0.41
1:B:151:VAL:HG23	1:B:152:LEU:HD12	2.02	0.41
1:A:70:MET:HE2	1:A:116:HIS:HE1	1.85	0.40
1:A:8:VAL:HG12	1:A:30:LEU:HD11	2.02	0.40
1:A:160:ARG:O	1:A:164:ASP:OD2	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:358:HOH:O	4:A:398:HOH:O[3_554]	2.13	0.07

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	189/192 (98%)	185 (98%)	4 (2%)	0	100	100
1	B	187/192 (97%)	175 (94%)	8 (4%)	4 (2%)	5	0
All	All	376/384 (98%)	360 (96%)	12 (3%)	4 (1%)	11	3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	ILE
1	B	105	ILE
1	B	141	PRO
1	B	155	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/154 (98%)	148 (98%)	3 (2%)	48	32
1	B	144/154 (94%)	140 (97%)	4 (3%)	38	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	295/308 (96%)	288 (98%)	7 (2%)	43 25

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	HIS
1	B	30	LEU
1	B	128	THR
1	B	186	THR
1	A	23	HIS
1	A	58	ASP
1	A	146	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	ASN
1	A	3	ASN

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 ⓘ

9 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	$\# Z > 2$
2	O0J	B	201	-	17,17,17	0.15	0	23,23,23	0.32	0
3	SO4	A	204	-	4,4,4	0.26	0	6,6,6	0.10	0
2	O0J	A	201	-	17,17,17	0.17	0	23,23,23	0.29	0
3	SO4	A	202	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	B	203	-	4,4,4	0.27	0	6,6,6	0.14	0
3	SO4	B	205	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	203	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	B	204	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	B	202	-	4,4,4	0.22	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	O0J	B	201	-	-	0/8/8/8	0/2/2/2
2	O0J	A	201	-	-	0/8/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

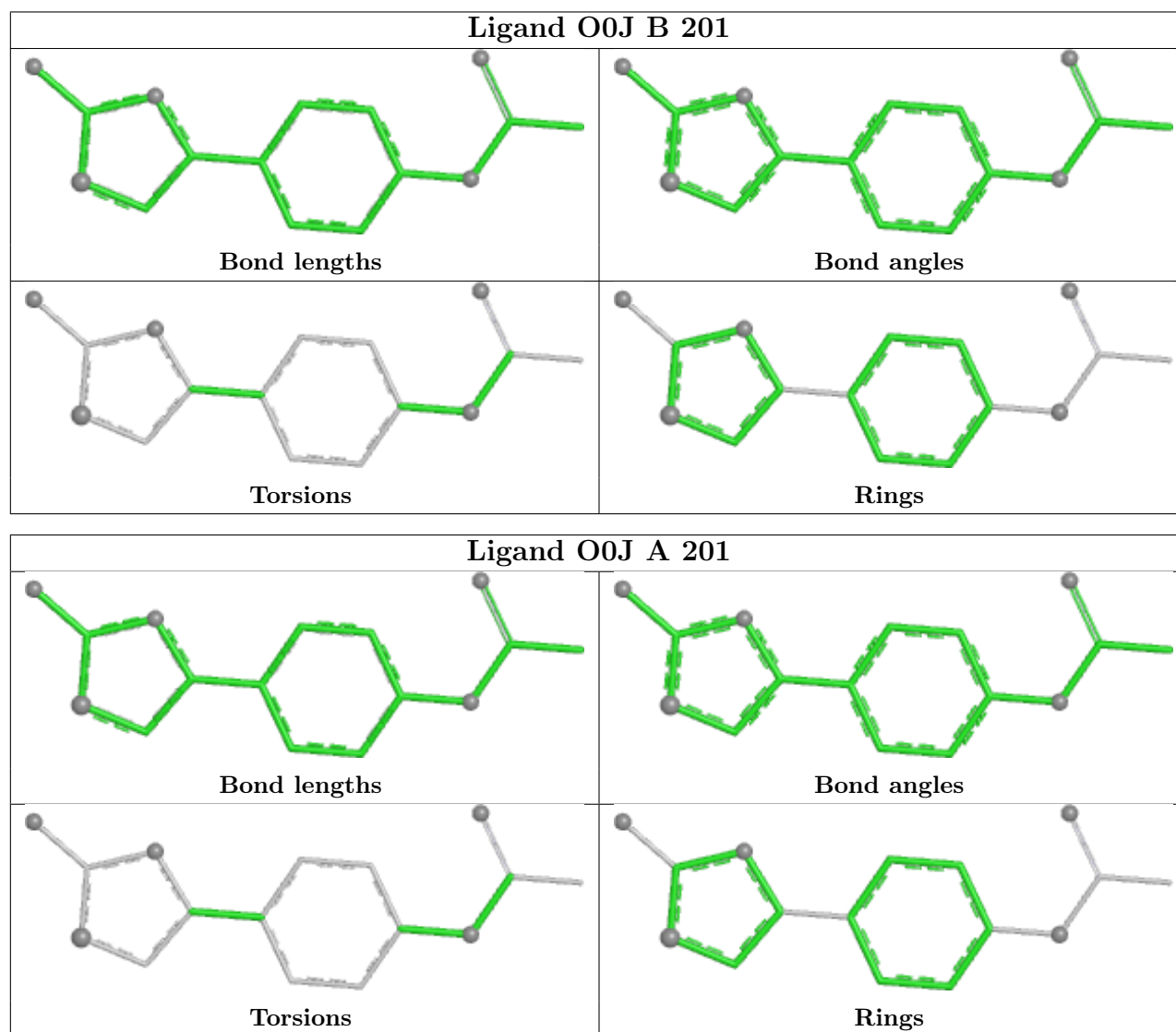
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	O0J	1	0
3	A	202	SO4	2	0
3	B	202	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/192 (99%)	2.47	116 (60%) 0 0	22, 35, 50, 57	2 (1%)
1	B	189/192 (98%)	2.81	124 (65%) 0 0	23, 38, 63, 72	0
All	All	380/384 (98%)	2.64	240 (63%) 0 0	22, 37, 56, 72	2 (0%)

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	8.9
1	B	157	ALA	7.1
1	B	156	SER	6.9
1	B	103	GLY	6.7
1	B	163	ILE	6.4
1	B	177	ILE	6.3
1	B	105	ILE	6.2
1	B	185	ALA	5.9
1	B	182	TRP	5.8
1	B	59	GLY	5.6
1	B	141	PRO	5.3
1	A	178	ILE	5.3
1	A	157	ALA	5.2
1	B	188	PHE	5.1
1	B	174	VAL	5.1
1	A	146	LEU	5.0
1	B	33	LEU	5.0
1	B	186	THR	5.0
1	B	178	ILE	5.0
1	B	60	ASP	4.9
1	B	29	PHE	4.9
1	B	56	LEU	4.9
1	B	189	LEU	4.9
1	B	4	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	106	LYS	4.8
1	A	187	ARG	4.7
1	A	182	TRP	4.7
1	B	102	CYS	4.7
1	A	143	ASP	4.7
1	B	179	SER	4.7
1	B	109	LEU	4.7
1	A	174	VAL	4.6
1	B	173	ALA	4.6
1	B	107	PHE	4.5
1	B	167	VAL	4.4
1	B	183	GLU	4.4
1	A	68	THR	4.4
1	B	54	ALA	4.3
1	A	2	SER	4.3
1	B	100	ILE	4.3
1	A	18	TYR	4.3
1	B	191	SER	4.2
1	B	168	ALA	4.2
1	A	3	ASN	4.2
1	A	35	TRP	4.2
1	B	159	HIS	4.2
1	A	184	GLU	4.2
1	A	69	PHE	4.1
1	A	186	THR	4.1
1	A	76	ALA	4.1
1	B	101	PRO	4.1
1	B	161	ARG	4.0
1	A	163	ILE	4.0
1	A	54	ALA	4.0
1	B	143	ASP	4.0
1	A	56	LEU	3.9
1	A	148	VAL	3.9
1	B	37	TRP	3.9
1	A	166	ALA	3.9
1	A	151	VAL	3.9
1	A	57	PRO	3.8
1	A	17	GLU	3.8
1	B	190	HIS	3.8
1	A	115	GLY	3.8
1	A	185	ALA	3.8
1	B	165	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLY	3.8
1	B	172	GLN	3.8
1	A	161	ARG	3.8
1	B	104	ARG	3.7
1	B	35	TRP	3.7
1	B	98	LEU	3.6
1	B	55	ALA	3.6
1	B	176	ASP	3.6
1	A	180	GLY	3.6
1	A	147	VAL	3.6
1	A	66	PRO	3.6
1	B	164	ASP	3.6
1	B	39	ALA	3.6
1	A	55	ALA	3.6
1	A	67	ALA	3.6
1	B	132	TYR	3.6
1	B	111	GLY	3.6
1	A	188	PHE	3.6
1	B	52	ALA	3.6
1	A	156	SER	3.6
1	A	52	ALA	3.5
1	A	189	LEU	3.6
1	B	62	TRP	3.5
1	B	57	PRO	3.5
1	B	146	LEU	3.5
1	A	155	PRO	3.5
1	B	5	ILE	3.5
1	B	147	VAL	3.5
1	B	175	PRO	3.4
1	B	166	ALA	3.4
1	B	134	LEU	3.4
1	B	155	PRO	3.4
1	A	16	LYS	3.4
1	B	171	LEU	3.4
1	A	175	PRO	3.4
1	B	140	HIS	3.3
1	A	165	ASP	3.3
1	B	91	ILE	3.3
1	A	100	ILE	3.3
1	B	181	LYS	3.3
1	A	105	ILE	3.3
1	B	42	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	152	LEU	3.3
1	A	152	LEU	3.3
1	A	164	ASP	3.3
1	B	187	ARG	3.3
1	B	151	VAL	3.3
1	A	167	VAL	3.2
1	B	6	LYS	3.2
1	A	191	SER	3.2
1	A	37	TRP	3.2
1	A	84	TYR	3.2
1	A	142	GLY	3.2
1	A	183	GLU	3.2
1	A	4	THR	3.1
1	A	5	ILE	3.1
1	A	15	GLY	3.1
1	A	91	ILE	3.1
1	A	98	LEU	3.1
1	B	16	LYS	3.1
1	A	48	PHE	3.1
1	A	43	GLU	3.1
1	A	61	VAL	3.0
1	A	28	TRP	3.0
1	B	184	GLU	3.0
1	A	63	LEU	3.0
1	B	148	VAL	3.0
1	A	77	VAL	3.0
1	A	41	PHE	3.0
1	B	114	GLY	3.0
1	B	154	LYS	3.0
1	B	61	VAL	3.0
1	A	149	GLY	3.0
1	B	18	TYR	2.9
1	B	153	ASN	2.9
1	B	142	GLY	2.9
1	B	160	ARG	2.9
1	B	136	LEU	2.9
1	A	153	ASN	2.9
1	A	145	ASN	2.8
1	B	53	ARG	2.8
1	B	128	THR	2.8
1	B	108	LYS	2.8
1	A	42	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	13	ASN	2.8
1	B	144	ARG	2.8
1	B	28	TRP	2.8
1	B	162	GLN	2.8
1	B	119	LEU	2.8
1	B	138	ILE	2.8
1	A	122	ILE	2.8
1	B	34	ALA	2.7
1	B	139	GLY	2.7
1	A	179	SER	2.7
1	A	20	GLN	2.7
1	B	158	GLU	2.7
1	B	112	GLY	2.7
1	A	58	ASP	2.7
1	B	63	LEU	2.7
1	B	88	PRO	2.7
1	B	122	ILE	2.7
1	B	124	ALA	2.6
1	A	30	LEU	2.6
1	A	144	ARG	2.6
1	B	58	ASP	2.6
1	B	115	GLY	2.6
1	A	99	ASP	2.6
1	B	129	ALA	2.6
1	A	81	ALA	2.6
1	A	181	LYS	2.6
1	B	170	SER	2.6
1	B	84	TYR	2.6
1	B	150	TYR	2.6
1	A	33	LEU	2.6
1	B	26	GLY	2.6
1	A	111	GLY	2.6
1	B	169	LYS	2.5
1	A	114	GLY	2.5
1	A	190	HIS	2.5
1	B	86	ILE	2.5
1	A	32	GLU	2.5
1	A	150	TYR	2.4
1	A	119	LEU	2.4
1	A	159	HIS	2.4
1	B	106	LYS	2.4
1	A	72	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	2.4
1	A	171	LEU	2.4
1	A	53	ARG	2.4
1	A	71	ASN	2.4
1	B	8	VAL	2.4
1	A	154	LYS	2.4
1	B	126	LEU	2.3
1	A	39	ALA	2.3
1	A	78	ALA	2.3
1	B	95	HIS	2.3
1	B	38	LYS	2.3
1	A	62	TRP	2.3
1	A	172	GLN	2.3
1	A	177	ILE	2.3
1	B	20	GLN	2.3
1	A	29	PHE	2.3
1	A	83	PHE	2.3
1	A	138	ILE	2.3
1	B	41	PHE	2.2
1	B	137	GLY	2.2
1	A	25	ALA	2.2
1	A	108	LYS	2.2
1	A	104	ARG	2.2
1	B	40	SER	2.2
1	A	27	PHE	2.2
1	B	113	ASN	2.2
1	B	127	GLY	2.2
1	A	14	PRO	2.2
1	A	173	ALA	2.2
1	B	43	GLU	2.2
1	A	92	LEU	2.2
1	A	141	PRO	2.2
1	A	50	GLU	2.1
1	B	110	GLY	2.1
1	A	49	GLY	2.1
1	A	45	LYS	2.1
1	B	25	ALA	2.1
1	A	129	ALA	2.1
1	B	51	VAL	2.1
1	A	134	LEU	2.1
1	A	120	LYS	2.0
1	B	21	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	93	VAL	2.0
1	A	19	GLU	2.0
1	A	23	HIS	2.0
1	B	149	GLY	2.0
1	B	131	TYR	2.0
1	A	51	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

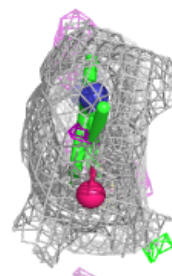
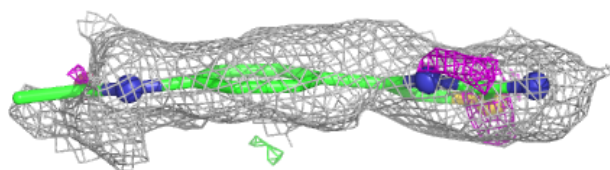
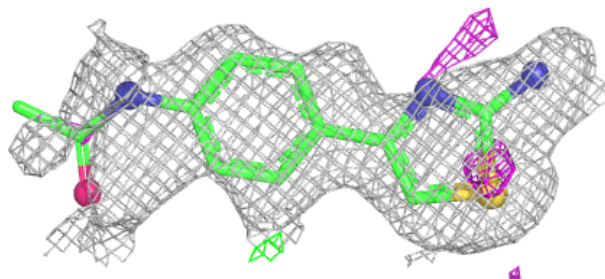
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	202	5/5	0.37	0.22	67,73,77,98	0
3	SO4	B	203	5/5	0.44	0.20	53,56,72,77	0
3	SO4	B	205	5/5	0.50	0.18	53,62,72,74	0
3	SO4	A	204	5/5	0.56	0.19	50,61,72,74	0
3	SO4	B	204	5/5	0.58	0.17	46,46,58,64	0
3	SO4	A	203	5/5	0.69	0.16	43,49,54,59	0
2	O0J	A	201	16/16	0.71	0.18	34,39,49,49	0
3	SO4	A	202	5/5	0.71	0.15	40,41,47,59	0
2	O0J	B	201	16/16	0.79	0.16	29,36,38,44	0

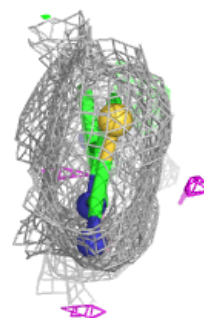
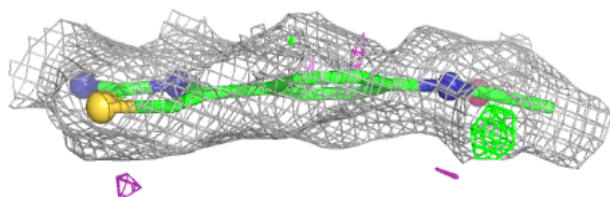
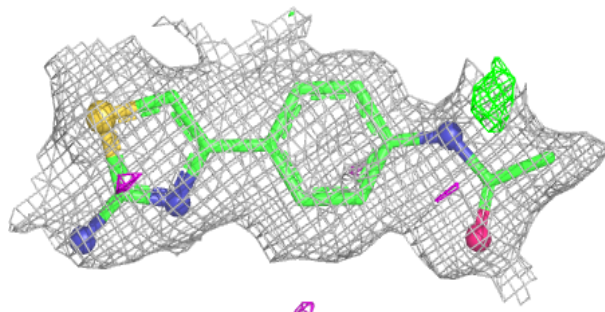
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around O0J A 201:

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

**Electron density around O0J B 201:**

$2mF_o-DF_c$ (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.