



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:38 PM UTC

PDB ID : 9O28 / pdb_00009o28
Title : Heparanase P6 in complex with fragment J59
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Deposited on : 2025-04-03
Resolution : 1.81 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

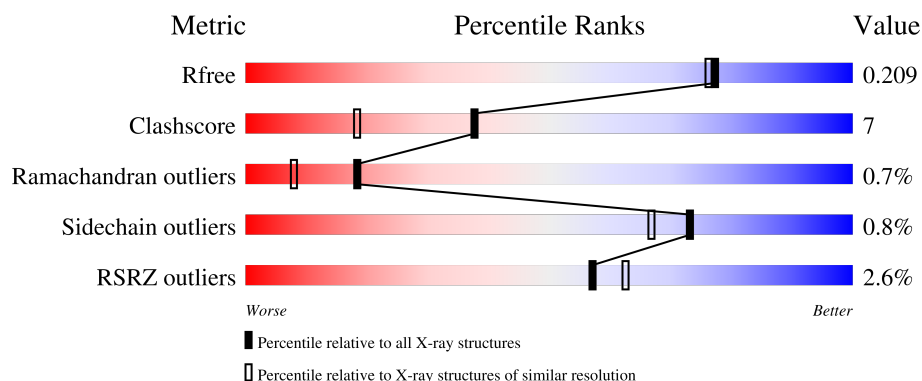
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 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	384	3% 88% 11%
2	B	74	85% 15%

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	EDO	A	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4058 atoms, of which 20 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 Heparanase 50 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	1	0
			3036	1957	522	547	10			

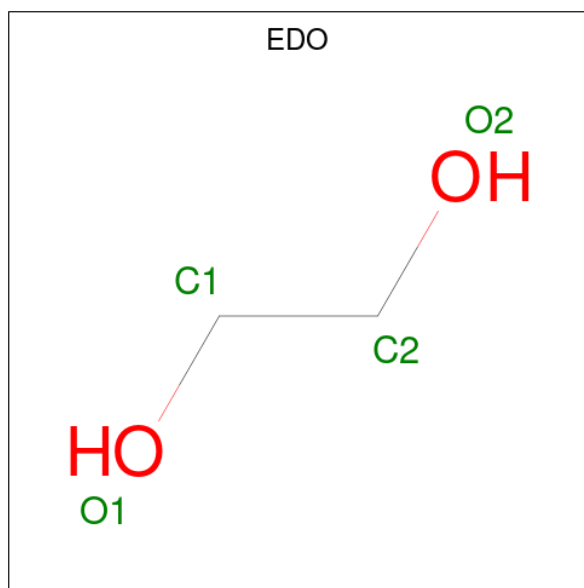
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LYS	ASN	conflict	UNP Q9Y251
A	195	SER	ALA	conflict	UNP Q9Y251
A	197	GLY	LEU	conflict	UNP Q9Y251
A	212	ALA	SER	conflict	UNP Q9Y251
A	219	ASP	SER	conflict	UNP Q9Y251
A	230	ARG	LEU	conflict	UNP Q9Y251
A	234	GLY	ASP	conflict	UNP Q9Y251
A	244	LYS	GLU	conflict	UNP Q9Y251
A	248	HIS	GLN	conflict	UNP Q9Y251
A	273	GLY	ARG	conflict	UNP Q9Y251
A	292	ALA	SER	conflict	UNP Q9Y251
A	307	LEU	LYS	conflict	UNP Q9Y251
A	318	THR	ILE	conflict	UNP Q9Y251
A	322	GLN	SER	conflict	UNP Q9Y251
A	327	LEU	PHE	conflict	UNP Q9Y251
A	354	GLY	LEU	conflict	UNP Q9Y251
A	426	GLN	SER	conflict	UNP Q9Y251
A	427	ASP	LYS	conflict	UNP Q9Y251
A	477	GLN	LYS	conflict	UNP Q9Y251
A	483	HIS	LEU	conflict	UNP Q9Y251
A	486	ASP	HIS	conflict	UNP Q9Y251
A	498	GLN	LEU	conflict	UNP Q9Y251
A	512	LYS	MET	conflict	UNP Q9Y251
A	513	PRO	GLU	conflict	UNP Q9Y251
A	530	ALA	SER	conflict	UNP Q9Y251
A	540	PRO	ALA	conflict	UNP Q9Y251

- Molecule 2 is a protein called Heparanase 8 kDa subunit.

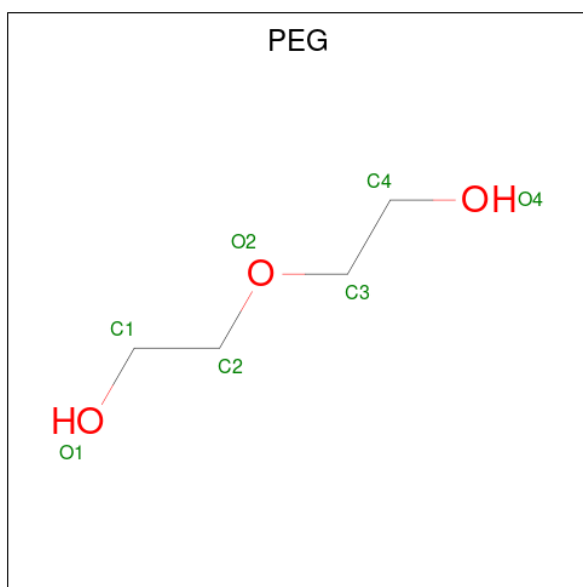
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	0	1	0
			594	388	98	108			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



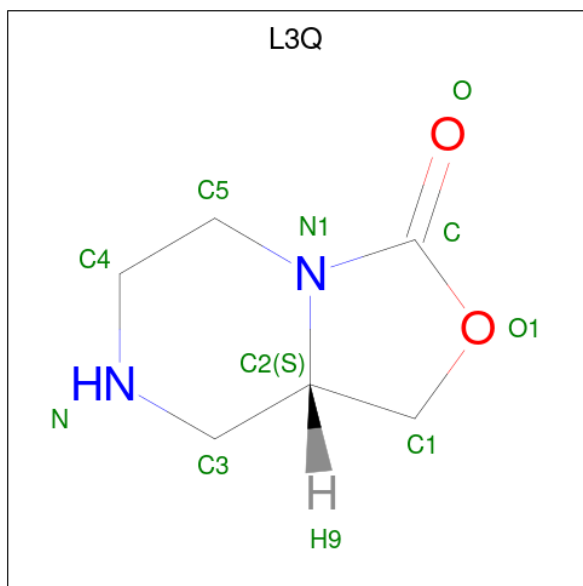
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



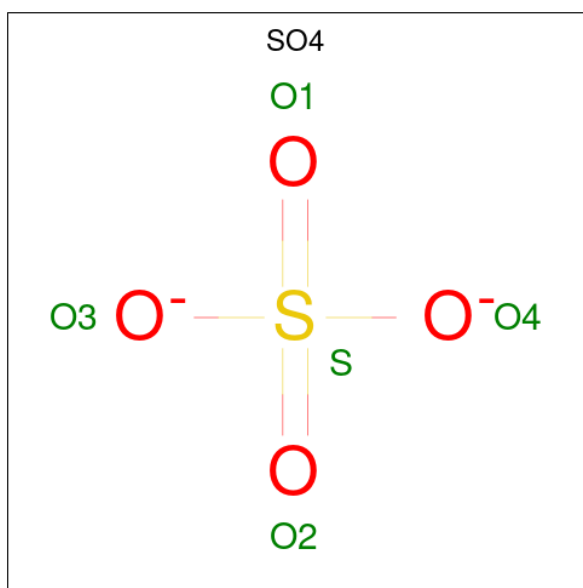
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			7	4	3			

- Molecule 5 is (8 {a} {S})-1,5,6,7,8,8 {a}-hexahydro-[1,3]oxazolo[3,4-a]pyrazin-3-one (CCD ID: L3Q) (formula: C₆H₁₀N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			20	6	10	2	2		
5	B	1	Total	C	H	N	O	0	0
			20	6	10	2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

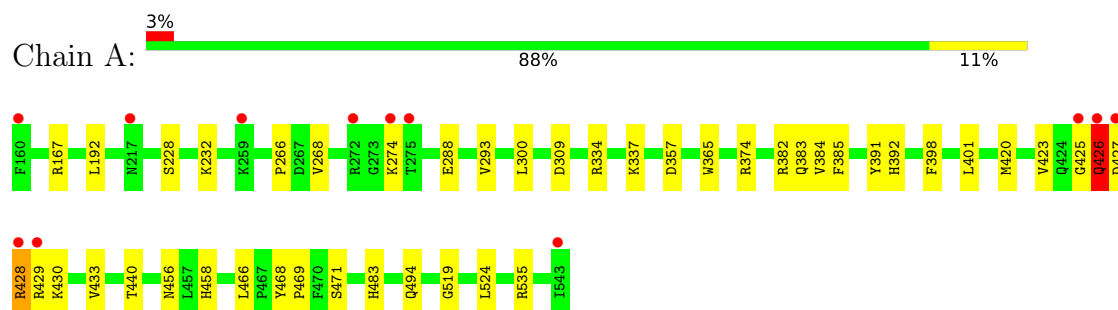
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	283	Total	O	0	0
			283	283		
7	B	67	Total	O	0	0
			67	67		

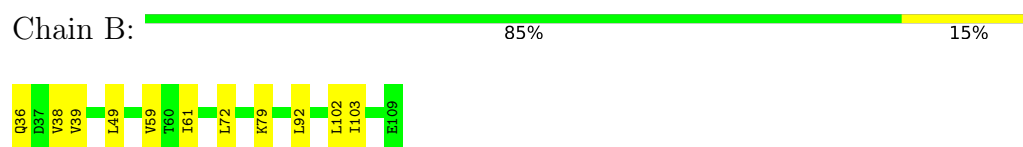
3 Residue-property plots

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: Heparanase 50 kDa subunit



- Molecule 2: Heparanase 8 kDa subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.87Å 74.97Å 124.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 1.81 46.30 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.30-1.81) 99.1 (46.30-1.81)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.178 , 0.210 0.178 , 0.209	Depositor DCC
R_{free} test set	2612 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4058	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: L3Q, SO4, PEG, EDO

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	0.28	0/3115	0.50	0/4218
2	B	0.29	0/611	0.44	0/828
All	All	0.28	0/3726	0.49	0/5046

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	3036	0	3057	46	0
2	B	594	0	610	16	0
3	A	16	0	24	8	0
4	A	7	0	10	2	0
5	A	10	10	0	3	0
5	B	10	10	0	0	0
6	A	15	0	0	0	0
7	A	283	0	0	2	0
7	B	67	0	0	0	0
All	All	4038	20	3701	52	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 7.

All (52) 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:420:MET:HE2	2:B:49:LEU:HD21	1.63	0.81
1:A:423:VAL:HG13	2:B:39:VAL:HG13	1.63	0.79
1:A:167:ARG:HH22	4:A:605:PEG:H22	1.52	0.75
1:A:483:HIS:HB2	1:A:494:GLN:HG3	1.74	0.69
1:A:420:MET:HE2	2:B:49:LEU:HD11	1.73	0.69
1:A:192:LEU:HD21	2:B:103:ILE:HD11	1.79	0.64
1:A:420:MET:CE	2:B:49:LEU:HD11	2.29	0.63
1:A:374:ARG:NH1	1:A:420:MET:HG3	2.14	0.62
1:A:423:VAL:HG13	2:B:39:VAL:CG1	2.31	0.61
1:A:266:PRO:HG2	1:A:268:VAL:HG13	1.83	0.60
1:A:535:ARG:NH1	3:A:603:EDO:H21	2.18	0.57
1:A:433:VAL:O	3:A:602:EDO:H21	2.03	0.57
2:B:36:GLN:HG3	2:B:38:VAL:H	1.68	0.57
1:A:423:VAL:CG1	2:B:39:VAL:HG13	2.33	0.57
1:A:420:MET:HE2	2:B:49:LEU:CD2	2.34	0.56
1:A:428:ARG:C	1:A:430:LYS:H	2.13	0.56
2:B:102:LEU:O	2:B:103:ILE:HD13	2.05	0.56
1:A:288:GLU:H	5:A:606:L3Q:C1	2.19	0.55
3:A:602:EDO:H12	7:A:729:HOH:O	2.08	0.54
1:A:483:HIS:CE1	3:A:601:EDO:H11	2.43	0.54
1:A:288:GLU:HB3	5:A:606:L3Q:O1	2.07	0.54
1:A:433:VAL:H	3:A:602:EDO:H11	1.73	0.53
1:A:420:MET:CE	2:B:49:LEU:HD21	2.36	0.53
1:A:535:ARG:HH11	3:A:603:EDO:H21	1.72	0.53
1:A:357:ASP:HB2	1:A:401:LEU:HD22	1.91	0.52
1:A:274:LYS:O	1:A:274:LYS:HE3	2.10	0.51
1:A:334:ARG:HH22	5:A:606:L3Q:C3	2.26	0.49
1:A:420:MET:HE2	2:B:49:LEU:CD1	2.42	0.49
1:A:466:LEU:O	1:A:471:SER:HB3	2.12	0.49
1:A:228:SER:OG	1:A:232:LYS:HE2	2.13	0.48
1:A:374:ARG:HH12	1:A:420:MET:HG3	1.76	0.48
1:A:428:ARG:NH2	1:A:458:HIS:HD2	2.12	0.47
1:A:433:VAL:H	3:A:602:EDO:C1	2.27	0.47
1:A:456:ASN:HB2	1:A:524:LEU:HD23	1.97	0.46
1:A:471:SER:O	1:A:519:GLY:HA2	2.16	0.46
4:A:605:PEG:H22	4:A:605:PEG:H41	1.72	0.46
1:A:425:GLY:O	1:A:426:GLN:HB2	2.15	0.45
1:A:427:ASP:O	1:A:428:ARG:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LEU:HD12	2:B:72:LEU:N	2.31	0.45
2:B:61:ILE:HG13	2:B:92:LEU:HD11	1.99	0.44
1:A:428:ARG:O	1:A:430:LYS:N	2.45	0.43
1:A:423:VAL:HG11	1:A:427:ASP:OD1	2.18	0.43
1:A:398:PHE:O	2:B:79:LYS:HE2	2.18	0.43
1:A:365:TRP:CH2	1:A:382:ARG:HB2	2.54	0.42
1:A:428:ARG:NH1	1:A:430:LYS:NZ	2.67	0.42
1:A:293:VAL:HG23	1:A:337:LYS:HG2	2.02	0.42
1:A:300:LEU:HD11	1:A:309:ASP:HB3	2.01	0.41
1:A:440:THR:HA	7:A:719:HOH:O	2.19	0.41
1:A:468:TYR:CG	1:A:469:PRO:HA	2.56	0.41
1:A:383:GLN:HA	1:A:384:VAL:HA	1.92	0.41
1:A:385:PHE:HB2	2:B:59:VAL:HB	2.02	0.41
1:A:483:HIS:HE1	3:A:601:EDO:H11	1.85	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	383/384 (100%)	369 (96%)	11 (3%)	3 (1%)	16	6
2	B	73/74 (99%)	72 (99%)	1 (1%)	0	100	100
All	All	456/458 (100%)	441 (97%)	12 (3%)	3 (1%)	18	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	ARG
1	A	429	ARG
1	A	426	GLN

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	330/329 (100%)	327 (99%)	3 (1%)	70	62
2	B	67/66 (102%)	67 (100%)	0	100	100
All	All	397/395 (100%)	394 (99%)	3 (1%)	73	67

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	TYR
1	A	392	HIS
1	A	426	GLN

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

Mol	Chain	Res	Type
1	A	260	ASN
1	A	426	GLN
1	A	458	HIS
1	A	474	GLN
1	A	483	HIS
2	B	64	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	604	-	3,3,3	0.23	0	2,2,2	0.34	0
6	SO4	A	609	-	4,4,4	0.68	0	6,6,6	0.26	0
3	EDO	A	603	-	3,3,3	0.28	0	2,2,2	0.15	0
4	PEG	A	605	-	6,6,6	0.25	0	5,5,5	0.23	0
5	L3Q	B	201	-	11,11,11	4.20	6 (54%)	11,15,15	3.78	6 (54%)
5	L3Q	A	606	-	11,11,11	4.27	6 (54%)	11,15,15	3.95	5 (45%)
3	EDO	A	601	-	3,3,3	0.24	0	2,2,2	0.41	0
3	EDO	A	602	-	3,3,3	0.25	0	2,2,2	0.20	0
6	SO4	A	607	-	4,4,4	0.71	0	6,6,6	0.10	0
6	SO4	A	608	-	4,4,4	0.68	0	6,6,6	0.05	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
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
4	PEG	A	605	-	-	2/4/4/4	-
5	L3Q	B	201	-	-	-	0/2/2/2
5	L3Q	A	606	-	-	-	0/2/2/2
3	EDO	A	601	-	-	1/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	L3Q	O1-C	9.17	1.46	1.35
5	B	201	L3Q	O1-C	8.91	1.46	1.35
5	B	201	L3Q	C-N1	7.94	1.49	1.35
5	A	606	L3Q	C-N1	7.92	1.49	1.35
5	A	606	L3Q	C2-N1	-4.69	1.40	1.47
5	B	201	L3Q	C2-N1	-4.56	1.40	1.47
5	A	606	L3Q	C3-C2	3.97	1.56	1.52
5	B	201	L3Q	C3-C2	3.93	1.56	1.52
5	B	201	L3Q	C5-N1	-2.40	1.42	1.47
5	A	606	L3Q	C5-N1	-2.26	1.43	1.47
5	A	606	L3Q	O1-C1	-2.14	1.41	1.45
5	B	201	L3Q	O1-C1	-2.10	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	L3Q	C1-C2-N1	8.57	107.95	100.40
5	B	201	L3Q	C1-C2-N1	7.70	107.19	100.40
5	A	606	L3Q	C5-N1-C	7.66	135.03	123.84
5	B	201	L3Q	C5-N1-C	7.39	134.64	123.84
5	A	606	L3Q	O1-C-O	3.39	126.57	122.53
5	B	201	L3Q	O1-C-O	3.26	126.41	122.53
5	B	201	L3Q	O1-C-N1	-3.03	107.73	109.87
5	B	201	L3Q	C3-C2-C1	-2.97	110.47	116.16
5	A	606	L3Q	O1-C-N1	-2.79	107.90	109.87
5	A	606	L3Q	C3-C2-C1	-2.75	110.89	116.16
5	B	201	L3Q	C1-O1-C	-2.49	107.22	109.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	PEG	O2-C3-C4-O4
4	A	605	PEG	C4-C3-O2-C2
3	A	602	EDO	O1-C1-C2-O2
3	A	601	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 13 short contacts:

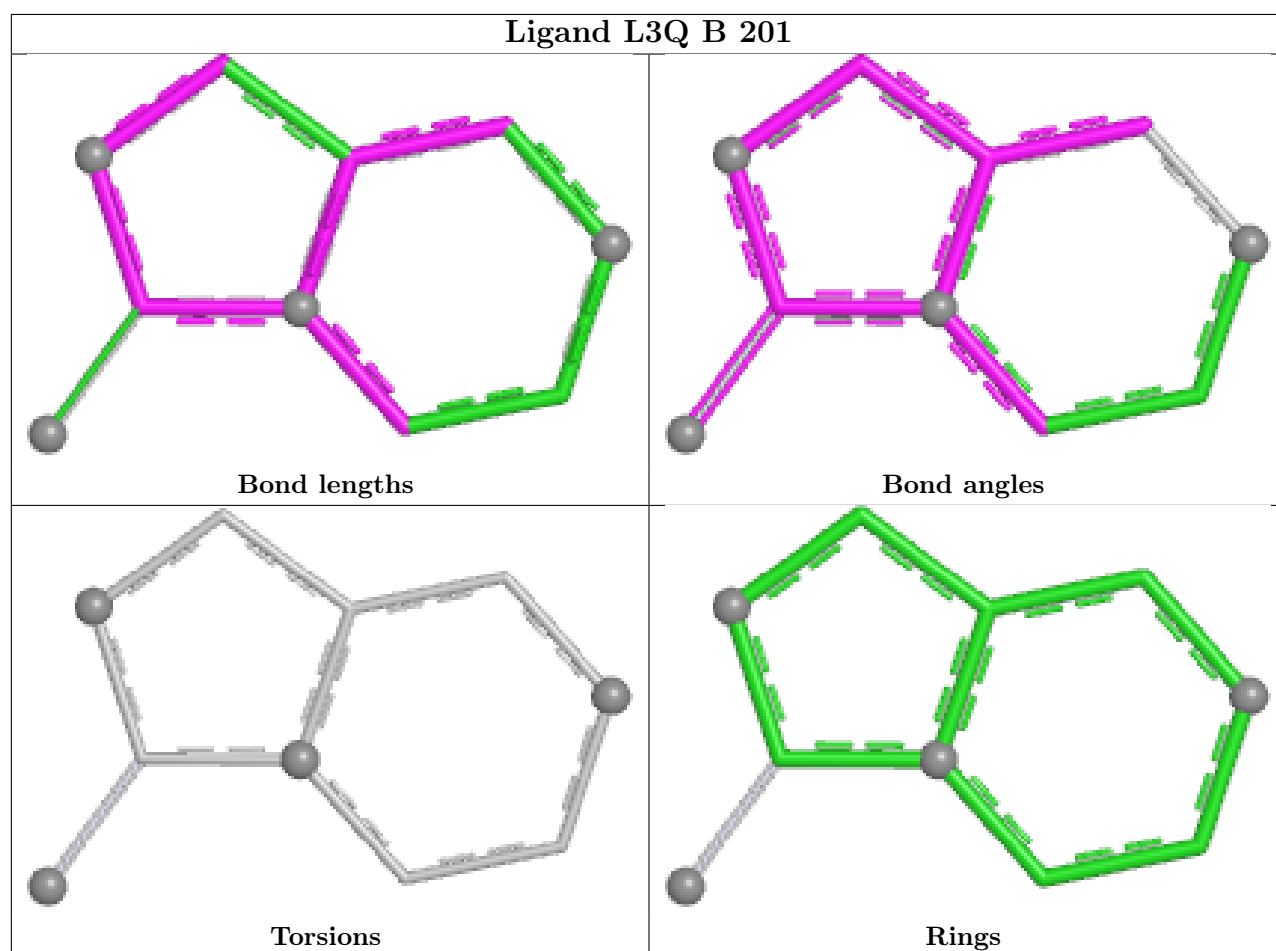
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	EDO	2	0

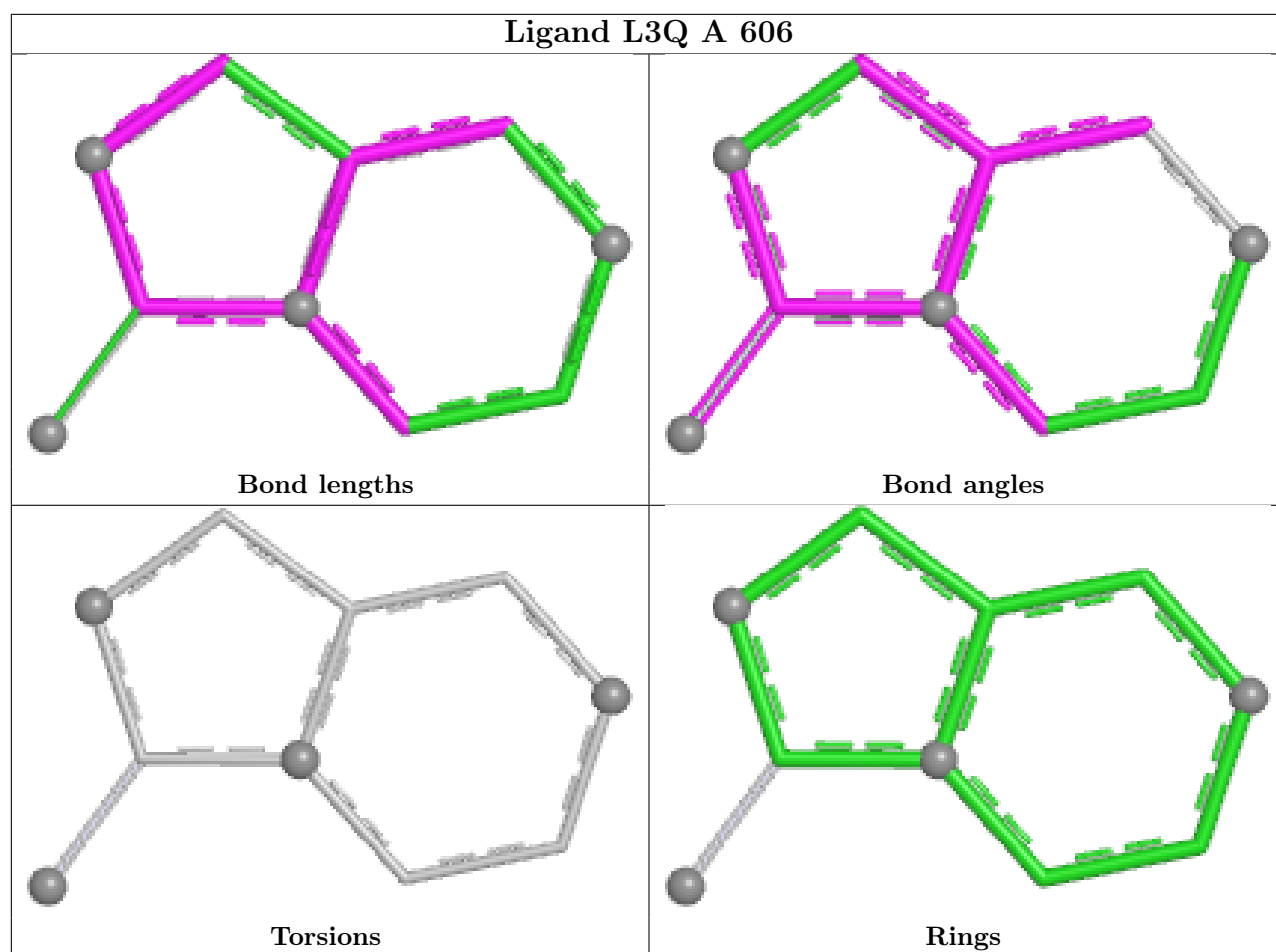
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	PEG	2	0
5	A	606	L3Q	3	0
3	A	601	EDO	2	0
3	A	602	EDO	4	0

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	384/384 (100%)	0.09	12 (3%) 51 58	17, 26, 44, 66	1 (0%)
2	B	74/74 (100%)	-0.01	0 100 100	14, 24, 39, 55	1 (1%)
All	All	458/458 (100%)	0.08	12 (2%) 57 62	14, 26, 43, 66	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	ASP	6.8
1	A	428	ARG	4.9
1	A	543	ILE	4.9
1	A	160	PHE	4.3
1	A	274	LYS	4.2
1	A	275	THR	3.2
1	A	429	ARG	2.8
1	A	426	GLN	2.8
1	A	272	ARG	2.7
1	A	217	ASN	2.5
1	A	425	GLY	2.4
1	A	259	LYS	2.4

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

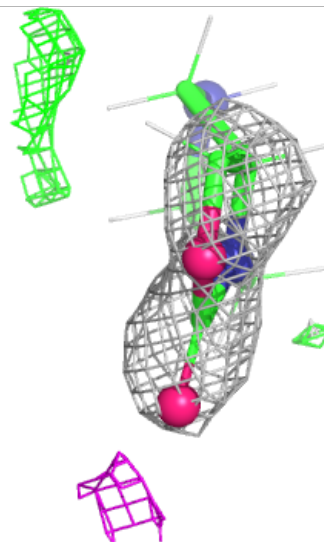
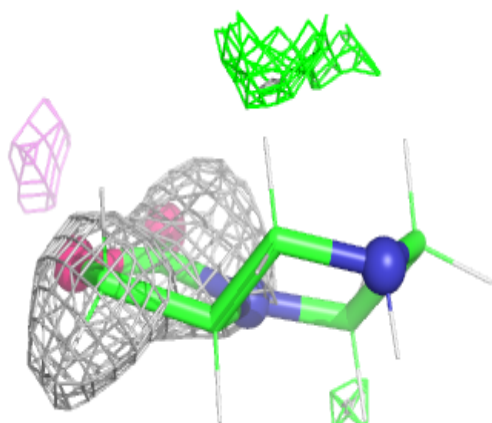
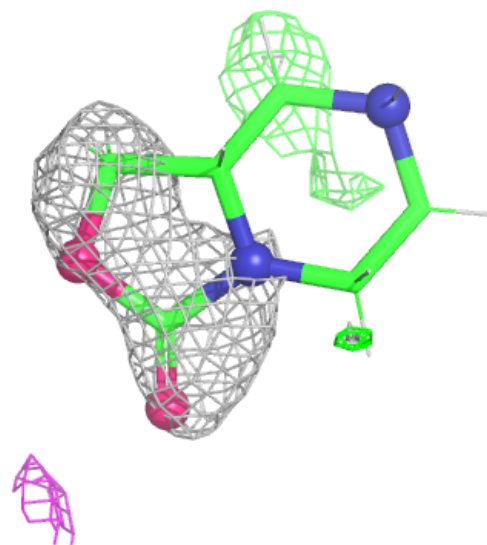
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	604	4/4	0.63	0.18	57,57,60,68	0
5	L3Q	A	606	10/10	0.67	0.23	43,61,76,79	20
4	PEG	A	605	7/7	0.70	0.17	53,53,57,63	0
3	EDO	A	603	4/4	0.72	0.17	46,47,51,52	0
3	EDO	A	601	4/4	0.73	0.16	47,48,54,55	0
6	SO4	A	607	5/5	0.76	0.14	36,38,44,44	5
6	SO4	A	608	5/5	0.80	0.14	42,43,49,56	5
5	L3Q	B	201	10/10	0.82	0.17	42,51,67,67	20
3	EDO	A	602	4/4	0.83	0.14	26,27,30,32	4
6	SO4	A	609	5/5	0.89	0.16	17,23,35,37	5

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.

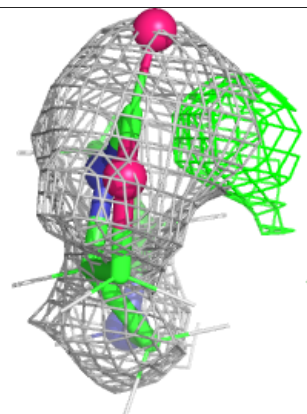
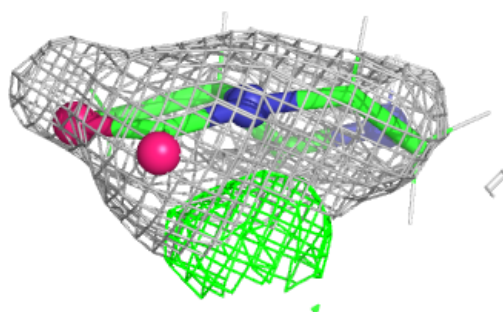
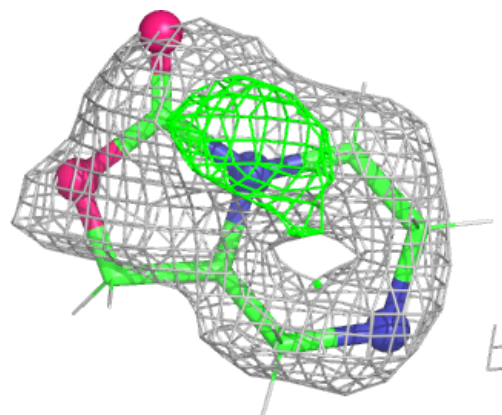
Electron density around L3Q A 606:

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



Electron density around L3Q 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 ⓘ

There are no such residues in this entry.