



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2025 – 06:22 pm BST

PDB ID : 9HJP / pdb_00009hjp
Title : Improved structure of mouse Gasdermin D
Authors : De Colibus, L.; Biasutto, A.; Jazayeri, A.; Duerr, K.L.
Deposited on : 2024-11-29
Resolution : 2.64 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

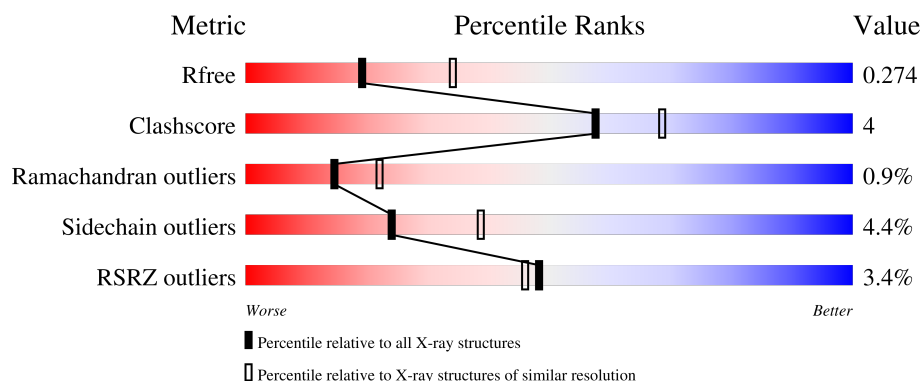
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	452	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	452	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6217 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 Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3139	1990	523	609	17			
1	B	386	Total	C	N	O	S	0	0	0
			3019	1920	502	581	16			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q9D8T2
A	?	-	GLY	deletion	UNP Q9D8T2
A	?	-	GLN	deletion	UNP Q9D8T2
A	?	-	PHE	deletion	UNP Q9D8T2
A	?	-	THR	deletion	UNP Q9D8T2
A	?	-	LEU	deletion	UNP Q9D8T2
A	?	-	GLY	deletion	UNP Q9D8T2
A	?	-	LYS	deletion	UNP Q9D8T2
A	?	-	GLY	deletion	UNP Q9D8T2
A	?	-	ARG	deletion	UNP Q9D8T2
A	?	-	LYS	deletion	UNP Q9D8T2
A	?	-	ALA	deletion	UNP Q9D8T2
A	?	-	VAL	deletion	UNP Q9D8T2
A	?	-	GLY	deletion	UNP Q9D8T2
A	?	-	GLN	deletion	UNP Q9D8T2
A	?	-	ARG	deletion	UNP Q9D8T2
A	?	-	HIS	deletion	UNP Q9D8T2
A	?	-	HIS	deletion	UNP Q9D8T2
A	?	-	GLY	deletion	UNP Q9D8T2
A	?	-	LEU	deletion	UNP Q9D8T2
A	?	-	ASN	deletion	UNP Q9D8T2
A	?	-	VAL	deletion	UNP Q9D8T2
A	?	-	LEU	deletion	UNP Q9D8T2
A	?	-	ALA	deletion	UNP Q9D8T2
A	?	-	ALA	deletion	UNP Q9D8T2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q9D8T2
A	?	-	CYS	deletion	UNP Q9D8T2
A	?	-	SER	deletion	UNP Q9D8T2
A	?	-	ILE	deletion	UNP Q9D8T2
A	?	-	GLY	deletion	UNP Q9D8T2
A	?	-	LYS	deletion	UNP Q9D8T2
A	?	-	GLN	deletion	UNP Q9D8T2
A	?	-	LEU	deletion	UNP Q9D8T2
A	?	-	SER	deletion	UNP Q9D8T2
A	?	-	LEU	deletion	UNP Q9D8T2
B	?	-	SER	deletion	UNP Q9D8T2
B	?	-	GLY	deletion	UNP Q9D8T2
B	?	-	GLN	deletion	UNP Q9D8T2
B	?	-	PHE	deletion	UNP Q9D8T2
B	?	-	THR	deletion	UNP Q9D8T2
B	?	-	LEU	deletion	UNP Q9D8T2
B	?	-	GLY	deletion	UNP Q9D8T2
B	?	-	LYS	deletion	UNP Q9D8T2
B	?	-	GLY	deletion	UNP Q9D8T2
B	?	-	ARG	deletion	UNP Q9D8T2
B	?	-	LYS	deletion	UNP Q9D8T2
B	?	-	ALA	deletion	UNP Q9D8T2
B	?	-	VAL	deletion	UNP Q9D8T2
B	?	-	GLY	deletion	UNP Q9D8T2
B	?	-	GLN	deletion	UNP Q9D8T2
B	?	-	ARG	deletion	UNP Q9D8T2
B	?	-	HIS	deletion	UNP Q9D8T2
B	?	-	HIS	deletion	UNP Q9D8T2
B	?	-	GLY	deletion	UNP Q9D8T2
B	?	-	LEU	deletion	UNP Q9D8T2
B	?	-	ASN	deletion	UNP Q9D8T2
B	?	-	VAL	deletion	UNP Q9D8T2
B	?	-	LEU	deletion	UNP Q9D8T2
B	?	-	ALA	deletion	UNP Q9D8T2
B	?	-	ALA	deletion	UNP Q9D8T2
B	?	-	LEU	deletion	UNP Q9D8T2
B	?	-	CYS	deletion	UNP Q9D8T2
B	?	-	SER	deletion	UNP Q9D8T2
B	?	-	ILE	deletion	UNP Q9D8T2
B	?	-	GLY	deletion	UNP Q9D8T2
B	?	-	LYS	deletion	UNP Q9D8T2
B	?	-	GLN	deletion	UNP Q9D8T2

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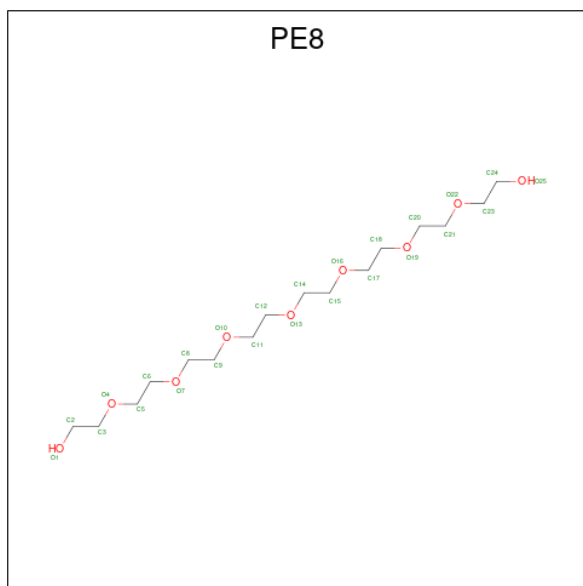
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP Q9D8T2
B	?	-	SER	deletion	UNP Q9D8T2
B	?	-	LEU	deletion	UNP Q9D8T2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	2	Total Cl 2 2	0	0

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 11 7 4	0	0

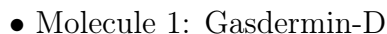
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Na 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	27	Total 27	O 27	0	0

- Molecule 1: Gasdermin-D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.21Å 86.93Å 82.47Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	33.95 – 2.64 33.95 – 2.64	Depositor EDS
% Data completeness (in resolution range)	59.1 (33.95-2.64) 59.1 (33.95-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.239 , 0.260 0.237 , 0.274	Depositor DCC
R_{free} test set	784 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6217	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PE8, NA, 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	0.59	0/3194	0.98	3/4330 (0.1%)
1	B	0.60	0/3073	0.97	1/4166 (0.0%)
All	All	0.60	0/6267	0.98	4/8496 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	5	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	455	GLU	N-CA-C	5.07	116.78	109.07
1	A	455	GLU	N-CA-C	5.00	116.68	109.07

There are no chirality outliers.

There are no planarity outliers.

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	3139	0	3176	28	0
1	B	3019	0	3065	30	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	B	11	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
5	A	15	0	0	0	0
5	B	27	0	0	0	0
All	All	6217	0	6254	55	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 4.

All (55) 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:116:SER:HB2	1:B:129:LYS:NZ	1.98	0.77
1:A:116:SER:HB2	1:B:129:LYS:HZ2	1.51	0.76
1:A:159:PHE:HB3	1:A:219:VAL:HG22	1.73	0.68
1:A:158:LEU:HD23	1:A:222:LEU:HD11	1.76	0.67
1:A:381:LEU:HD13	1:A:384:LEU:HD12	1.76	0.66
1:A:159:PHE:HB3	1:A:219:VAL:CG2	2.25	0.65
1:B:158:LEU:HD23	1:B:222:LEU:HD11	1.78	0.65
1:B:119:MET:HG3	1:B:171:VAL:HG21	1.79	0.64
1:A:424:VAL:HB	1:A:459:VAL:CG2	2.28	0.63
1:A:424:VAL:HB	1:A:459:VAL:HG22	1.80	0.62
1:B:377:LEU:HD13	1:B:478:LEU:HB2	1.83	0.61
1:A:29:LEU:HD21	1:A:209:ILE:HG23	1.82	0.60
1:A:377:LEU:HD13	1:A:478:LEU:HB2	1.83	0.59
1:A:119:MET:HG3	1:A:171:VAL:HG21	1.85	0.58
1:B:322:LEU:HD21	1:B:381:LEU:HD13	1.87	0.57
1:B:6:GLU:HG2	1:B:10:LYS:NZ	2.23	0.54
1:A:2:PRO:HB3	1:A:7:LYS:HB2	1.90	0.54
1:B:12:VAL:HG22	1:B:83:VAL:HG11	1.89	0.53
1:B:306:LEU:HB3	1:B:310:LEU:HD23	1.90	0.53
1:A:163:GLU:HB3	1:A:218:ARG:HB3	1.92	0.52
1:B:163:GLU:HB3	1:B:218:ARG:HB3	1.91	0.52
1:B:3:SER:HB3	1:B:6:GLU:HB3	1.91	0.52
1:B:139:HIS:CE1	1:B:142:GLN:NE2	2.77	0.52
1:A:426:LEU:HB3	1:A:430:LEU:HD21	1.93	0.51
1:A:7:LYS:HB3	1:A:88:ASP:HB3	1.94	0.50
1:A:321:ILE:HD12	1:A:328:MET:HG3	1.94	0.50
1:B:303:LEU:O	1:B:304:GLU:HB2	2.12	0.49
1:B:321:ILE:HD12	1:B:328:MET:HG3	1.93	0.49
1:A:29:LEU:HD11	1:A:209:ILE:HG12	1.95	0.48
1:B:411:VAL:HG23	1:B:426:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LEU:HD22	1:A:441:THR:HG21	1.95	0.47
1:A:306:LEU:HD21	1:A:370:LEU:HD21	1.95	0.47
1:B:360:VAL:HG23	1:B:366:LEU:HD23	1.96	0.47
1:A:12:VAL:HG22	1:A:83:VAL:HG21	1.96	0.47
1:B:1:MET:HE3	1:B:2:PRO:HD2	1.97	0.47
1:B:407:LEU:HD22	1:B:441:THR:HG21	1.96	0.47
1:A:360:VAL:HG23	1:A:366:LEU:HD23	1.97	0.46
1:B:316:VAL:HG22	1:B:320:LYS:HE3	1.98	0.45
1:B:174:THR:HG22	1:B:206:MET:HG3	1.99	0.44
1:B:359:LEU:HD21	1:B:374:ILE:HG13	1.99	0.44
1:A:359:LEU:HD21	1:A:374:ILE:HG13	1.99	0.43
1:B:9:VAL:HG22	1:B:215:LEU:HB3	2.00	0.43
1:B:407:LEU:HG	1:B:426:LEU:HD22	1.99	0.43
1:A:316:VAL:HG22	1:A:320:LYS:HE3	2.00	0.43
1:A:397:GLU:O	1:A:401:LEU:HB2	2.19	0.43
1:B:6:GLU:O	1:B:10:LYS:HG2	2.19	0.42
1:B:6:GLU:HG2	1:B:10:LYS:HZ1	1.83	0.42
1:A:407:LEU:HD21	1:A:430:LEU:HD22	2.01	0.41
1:A:116:SER:CB	1:B:129:LYS:NZ	2.76	0.41
1:B:410:HIS:ND1	1:B:427:PRO:HD3	2.36	0.41
1:B:81:PHE:HE1	1:B:123:ILE:HG13	1.86	0.41
1:B:377:LEU:O	1:B:381:LEU:HG	2.21	0.41
1:A:180:GLU:HG2	1:A:184:ALA:HB3	2.03	0.40
1:A:456:SER:HA	1:A:457:PRO:HA	1.94	0.40
1:B:445:LEU:HB2	1:B:452:LEU:HD11	2.03	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	396/452 (88%)	377 (95%)	14 (4%)	5 (1%)	10 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	378/452 (84%)	364 (96%)	12 (3%)	2 (0%)	25	37
All	All	774/904 (86%)	741 (96%)	26 (3%)	7 (1%)	14	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	288	ASP
1	A	144	GLU
1	B	144	GLU
1	A	456	SER
1	B	456	SER
1	A	429	VAL

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	361/397 (91%)	345 (96%)	16 (4%)	24	39
1	B	346/397 (87%)	331 (96%)	15 (4%)	25	40
All	All	707/794 (89%)	676 (96%)	31 (4%)	24	39

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	49	ARG
1	A	187	LEU
1	A	222	LEU
1	A	237	LYS
1	A	315	LEU
1	A	323	GLN
1	A	346	GLU
1	A	349	ASP

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Mol	Chain	Res	Type
1	A	360	VAL
1	A	370	LEU
1	A	381	LEU
1	A	397	GLU
1	A	437	GLU
1	A	459	VAL
1	A	464	THR
1	B	9	VAL
1	B	20	ARG
1	B	22	ASP
1	B	23	LEU
1	B	36	ARG
1	B	49	ARG
1	B	76	GLU
1	B	222	LEU
1	B	292	LEU
1	B	306	LEU
1	B	309	GLU
1	B	323	GLN
1	B	360	VAL
1	B	401	LEU
1	B	485	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	135	GLN
1	A	139	HIS
1	A	149	GLN
1	A	177	HIS
1	A	201	GLN
1	A	313	GLN
1	A	325	GLN
1	A	389	GLN
1	A	421	GLN
1	B	135	GLN
1	B	139	HIS
1	B	141	GLN
1	B	142	GLN
1	B	150	GLN
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	313	GLN
1	B	325	GLN
1	B	389	GLN
1	B	419	GLN
1	B	421	GLN
1	B	484	GLN

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](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
3	PE8	B	501	-	10,10,24	0.18	0	9,9,23	0.08	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	PE8	B	501	-	-	6/8/8/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

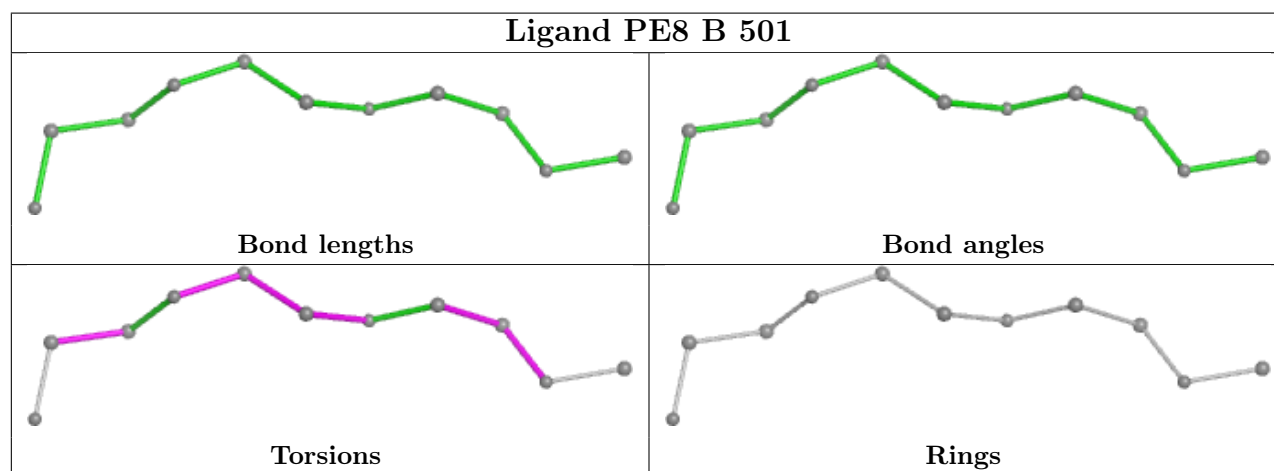
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	PE8	O16-C17-C18-O19
3	B	501	PE8	O22-C23-C24-O25
3	B	501	PE8	O19-C20-C21-O22
3	B	501	PE8	C20-C21-O22-C23
3	B	501	PE8	C18-C17-O16-C15
3	B	501	PE8	C21-C20-O19-C18

There are no ring outliers.

No monomer is involved in short contacts.

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	404/452 (89%)	0.61	22 (5%) 32 31	49, 104, 152, 184	0
1	B	386/452 (85%)	0.23	5 (1%) 74 73	41, 72, 105, 144	0
All	All	790/904 (87%)	0.42	27 (3%) 48 46	41, 86, 144, 184	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	SER	3.6
1	A	5	PHE	3.3
1	A	303	LEU	2.8
1	A	366	LEU	2.8
1	A	352	ALA	2.7
1	A	287	ALA	2.7
1	A	418	TRP	2.7
1	A	377	LEU	2.6
1	B	18	GLY	2.6
1	A	476	LEU	2.5
1	B	215	LEU	2.5
1	A	374	ILE	2.5
1	A	432	GLY	2.5
1	A	1	MET	2.4
1	A	21	GLY	2.4
1	A	430	LEU	2.3
1	A	81	PHE	2.3
1	A	4	ALA	2.3
1	A	356	LEU	2.3
1	B	207	VAL	2.2
1	B	117	ALA	2.2
1	A	173	ILE	2.2
1	A	381	LEU	2.2
1	A	398	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	361	LEU	2.1
1	A	399	THR	2.1
1	A	188	LYS	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](#)

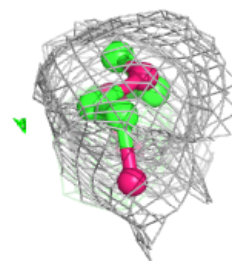
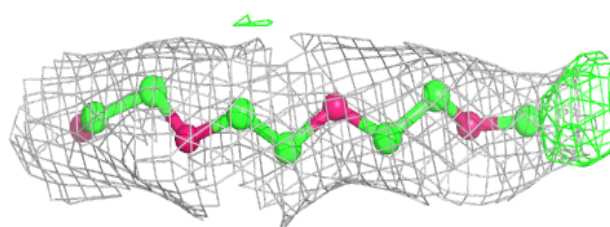
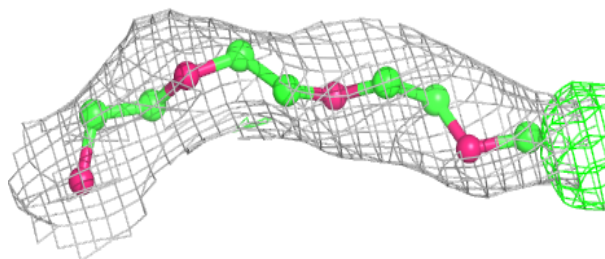
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PE8	B	501	11/25	0.71	0.12	96,96,96,96	0
4	NA	B	506	1/1	0.83	0.06	53,53,53,53	0
4	NA	B	505	1/1	0.91	0.17	69,69,69,69	0
2	CL	A	501	1/1	0.95	0.11	80,80,80,80	0
4	NA	B	503	1/1	0.96	0.17	49,49,49,49	0
2	CL	B	504	1/1	0.96	0.06	66,66,66,66	0
2	CL	B	502	1/1	0.96	0.05	67,67,67,67	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 PE8 B 501:

$2mF_o-DF_c$ (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.