



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2024 – 04:20 pm BST

PDB ID : 7R2M  
Title : SYNJ2BP complex with a synthetic Vangl2 peptide (9mer).  
Authors : Carrasco, K.; Cousido Siah, A.; Gogl, G.; Betzi, S.; McEwen, A.; Kostmann, C.; Trave, G.  
Deposited on : 2022-02-04  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

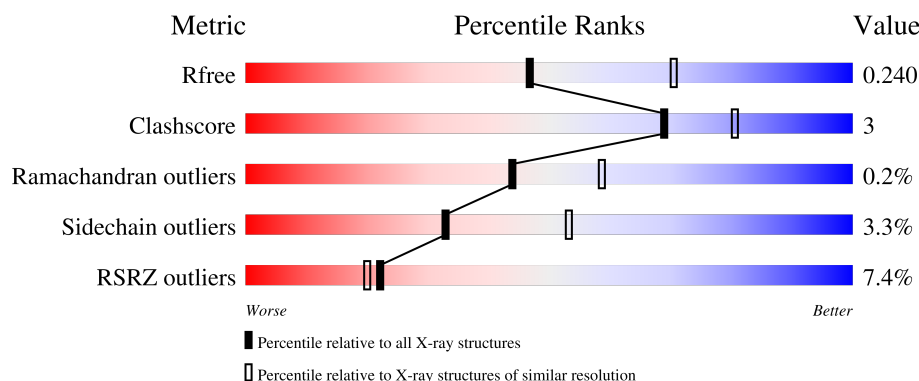
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	422	<div> <div>5%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	D	422	<div> <div>9%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
2	B	24	<div> <div>8%</div> <div>25%</div> <div>75%</div> </div>
2	E	24	<div> <div>12%</div> <div>25%</div> <div>75%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6861 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 Synaptojanin-2-binding protein,Annexin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	417	Total	C	N	O	S	0	2	0
			3322	2075	580	656	11			
1	A	417	Total	C	N	O	S	0	2	0
			3332	2082	584	655	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLN	-	expression tag	UNP P57105
D	2	GLY	-	expression tag	UNP P57105
D	3	SER	-	expression tag	UNP P57105
D	4	HIS	-	expression tag	UNP P57105
D	5	MET	-	expression tag	UNP P57105
D	104	GLY	-	linker	UNP P57105
D	243	ILE	VAL	conflict	UNP A0A4W2GEM6
D	306	PRO	CYS	conflict	UNP A0A4W2GEM6
D	313	ASP	GLU	conflict	UNP A0A4W2GEM6
D	328	ARG	LYS	conflict	UNP A0A4W2GEM6
D	392	ARG	LYS	conflict	UNP A0A4W2GEM6
A	1	GLN	-	expression tag	UNP P57105
A	2	GLY	-	expression tag	UNP P57105
A	3	SER	-	expression tag	UNP P57105
A	4	HIS	-	expression tag	UNP P57105
A	5	MET	-	expression tag	UNP P57105
A	104	GLY	-	linker	UNP P57105
A	243	ILE	VAL	conflict	UNP A0A4W2GEM6
A	306	PRO	CYS	conflict	UNP A0A4W2GEM6
A	313	ASP	GLU	conflict	UNP A0A4W2GEM6
A	328	ARG	LYS	conflict	UNP A0A4W2GEM6
A	392	ARG	LYS	conflict	UNP A0A4W2GEM6

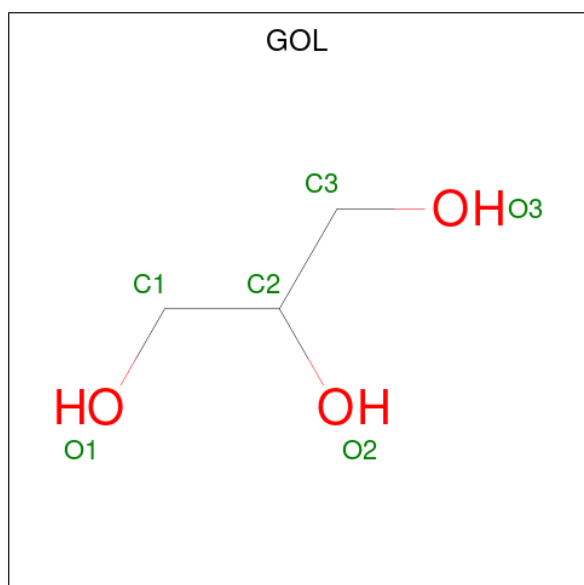
- Molecule 2 is a protein called Vangl2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			40	23	6	11			
2	E	6	Total	C	N	O	0	0	0
			40	23	6	11			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	5	Total	Ca	0	0
			5	5		
3	A	4	Total	Ca	0	0
			4	4		

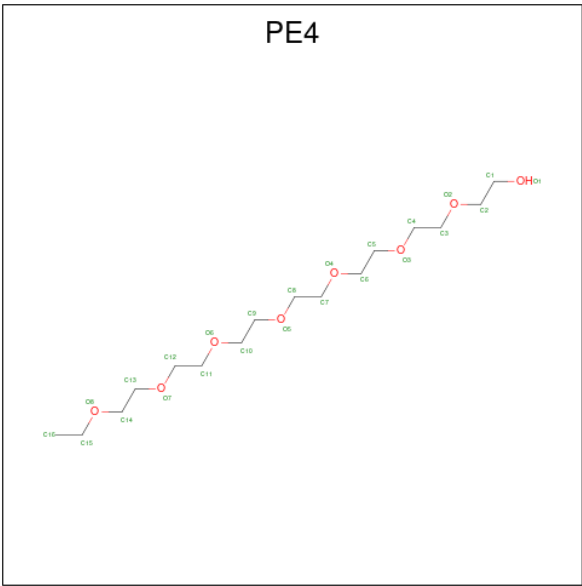
- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			14	10	4		

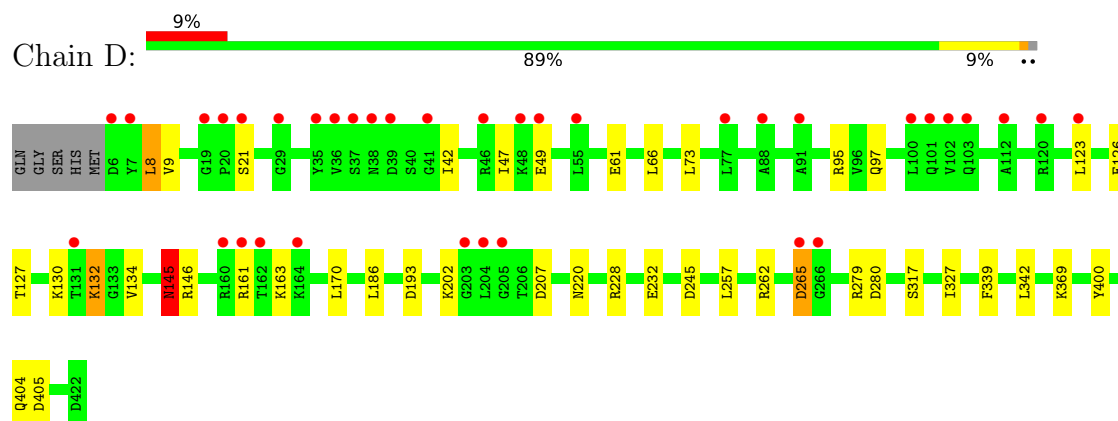
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	47	Total	O	0	0
			47	47		
6	A	33	Total	O	0	0
			33	33		

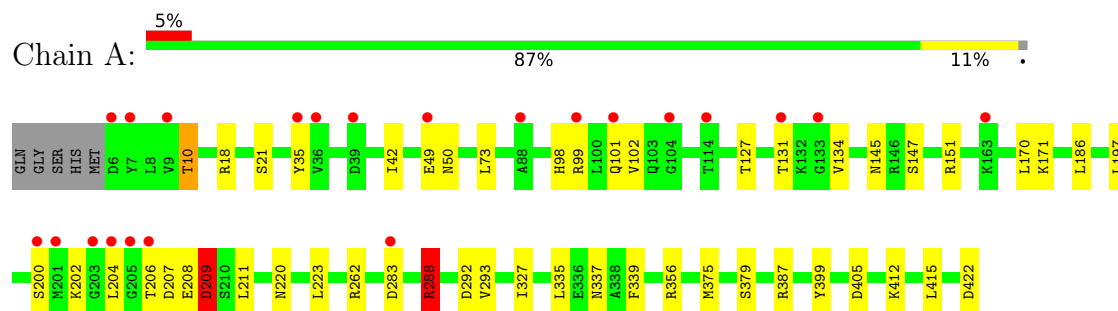
### 3 Residue-property plots [i](#)

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: Synaptojanin-2-binding protein,Annexin



- Molecule 1: Synaptojanin-2-binding protein,Annexin



- Molecule 2: Vangl2 peptide



- Molecule 2: Vangl2 peptide



GLY	SER	GLY	SER	GLY	SER	GLY	MET	ARG	LEU	Q201	S202	Y206	MET	ARG	LEU	GLN	SER	GLU	THR	SER	VAL
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.27Å 60.71Å 143.15Å 90.00° 92.88° 90.00°	Depositor
Resolution (Å)	47.66 – 2.40 47.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.66-2.40) 96.6 (47.66-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.215 , 0.239 0.215 , 0.240	Depositor DCC
$R_{free}$ test set	3366 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l 0.013 for k,h,-l 0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: PE4, CA, GOL

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	0.39	1/3375 (0.0%)	0.52	0/4536
1	D	0.43	2/3365 (0.1%)	0.52	2/4524 (0.0%)
2	B	0.68	0/39	0.76	0/52
2	E	0.68	0/39	0.86	0/52
All	All	0.41	3/6818 (0.0%)	0.52	2/9164 (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	A	0	4
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	145[A]	ASN	C-N	-9.53	1.12	1.34
1	D	145[B]	ASN	C-N	-9.53	1.12	1.34
1	A	223	LEU	C-N	-5.12	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145[A]	ASN	O-C-N	-5.01	114.69	122.70
1	D	145[B]	ASN	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	GLU	Mainchain
1	A	209[B]	ASP	Mainchain
1	A	288[B]	ARG	Mainchain
1	D	145[A]	ASN	Mainchain

## 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	3332	0	3341	20	2
1	D	3322	0	3317	26	2
2	B	40	0	33	0	0
2	E	40	0	33	0	0
3	A	4	0	0	0	0
3	D	5	0	0	0	0
4	A	12	0	16	0	0
4	D	12	0	16	0	0
5	D	14	0	16	1	0
6	A	33	0	0	2	0
6	D	47	0	0	7	0
All	All	6861	0	6772	46	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (46) 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:D:123:LEU:HB2	6:D:603:HOH:O	1.31	1.29
1:D:163:LYS:NZ	6:D:602:HOH:O	1.87	1.06
1:D:161:ARG:NH2	6:D:603:HOH:O	2.05	0.90
1:D:123:LEU:HD13	6:D:603:HOH:O	1.78	0.83
1:D:265[A]:ASP:OD2	1:D:265[A]:ASP:N	2.15	0.71
1:A:292:ASP:OD2	6:A:602:HOH:O	2.10	0.70
1:D:123:LEU:CD1	6:D:603:HOH:O	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:OG	1:A:207:ASP:HB3	2.00	0.62
1:D:161:ARG:CZ	6:D:603:HOH:O	2.44	0.60
1:D:327:ILE:HD13	1:D:339:PHE:HB3	1.87	0.56
1:A:170:LEU:HD12	1:A:186:LEU:HD11	1.87	0.56
1:D:145[A]:ASN:C	1:D:146:ARG:HG2	2.26	0.56
1:D:193:ASP:OD1	6:D:605:HOH:O	2.18	0.56
1:D:9:VAL:HG13	1:D:97:GLN:HG3	1.88	0.56
1:D:42:ILE:HG13	1:D:73:LEU:HD23	1.88	0.55
1:A:171:LYS:NZ	6:A:607:HOH:O	2.41	0.54
1:A:293:VAL:HG11	1:A:335:LEU:HD21	1.90	0.54
1:A:42:ILE:HG13	1:A:73:LEU:HD23	1.91	0.53
1:D:207:ASP:OD2	1:D:369:LYS:NZ	2.35	0.52
1:A:49:GLU:H	1:A:49:GLU:CD	2.13	0.52
1:A:283:ASP:O	1:A:288[A]:ARG:HG2	2.09	0.52
1:D:257:LEU:HD11	1:D:342:LEU:HD22	1.93	0.51
1:D:279:ARG:NH2	5:D:507:PE4:H52	2.27	0.48
1:D:47:ILE:HG13	1:D:61:GLU:HG2	1.96	0.48
1:D:170:LEU:HD12	1:D:186:LEU:HD11	1.96	0.48
1:A:387:ARG:HB3	1:A:422:ASP:OD2	2.14	0.48
1:A:327:ILE:HD13	1:A:339:PHE:HB3	1.98	0.46
1:A:220:ASN:ND2	1:A:262:ARG:O	2.48	0.46
1:D:132:LYS:HB3	1:D:132:LYS:HE3	1.78	0.44
1:D:66:LEU:HD12	1:D:95:ARG:HG2	2.00	0.44
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.83	0.44
1:A:10:THR:HG23	1:A:98:HIS:HB2	1.98	0.44
1:A:127:THR:O	1:A:131:THR:HG23	2.18	0.44
1:D:8:LEU:HD12	1:D:8:LEU:HA	1.79	0.44
1:D:49:GLU:H	1:D:49:GLU:CD	2.20	0.44
1:D:400:TYR:O	1:D:404:GLN:HG2	2.19	0.43
1:A:399:TYR:CD2	1:A:415:LEU:HD22	2.54	0.43
1:A:200:SER:HG	1:A:207:ASP:HB3	1.85	0.42
1:A:147:SER:O	1:A:151:ARG:HG3	2.19	0.42
1:A:375:MET:O	1:A:379:SER:HB3	2.20	0.42
1:D:228:ARG:O	1:D:232:GLU:HG3	2.20	0.41
1:A:49:GLU:O	1:A:50:ASN:HB2	2.21	0.41
1:A:209[A]:ASP:OD1	1:A:356:ARG:NH2	2.34	0.41
1:D:220:ASN:ND2	1:D:262:ARG:O	2.52	0.40
1:D:126:GLU:O	1:D:127:THR:C	2.58	0.40
1:A:197:LEU:HD22	1:A:211:LEU:HD12	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLU:OE2	1:A:50:ASN:ND2[2_554]	1.80	0.40
1:D:280:ASP:OD1	1:A:18:ARG:NH2[1_565]	2.07	0.13

## 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	417/422 (99%)	409 (98%)	7 (2%)	1 (0%)	44	59
1	D	417/422 (99%)	409 (98%)	7 (2%)	1 (0%)	44	59
2	B	4/24 (17%)	4 (100%)	0	0	100	100
2	E	4/24 (17%)	4 (100%)	0	0	100	100
All	All	842/892 (94%)	826 (98%)	14 (2%)	2 (0%)	44	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	VAL
1	D	134	VAL

### 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	361/364 (99%)	344 (95%)	17 (5%)	22	38
1	D	359/364 (99%)	349 (97%)	10 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	5/20 (25%)	5 (100%)	0	100	100
2	E	5/20 (25%)	5 (100%)	0	100	100
All	All	730/768 (95%)	703 (96%)	27 (4%)	33	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	8	LEU
1	D	21	SER
1	D	130	LYS
1	D	132	LYS
1	D	202	LYS
1	D	245	ASP
1	D	265[A]	ASP
1	D	265[B]	ASP
1	D	317	SER
1	D	405	ASP
1	A	10	THR
1	A	21	SER
1	A	35	TYR
1	A	99	ARG
1	A	101	GLN
1	A	102	VAL
1	A	145	ASN
1	A	202	LYS
1	A	204	LEU
1	A	206	THR
1	A	209[A]	ASP
1	A	209[B]	ASP
1	A	288[A]	ARG
1	A	288[B]	ARG
1	A	337	ASN
1	A	405	ASP
1	A	412	LYS

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

Mol	Chain	Res	Type
1	D	34	GLN
1	A	34	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	$\# Z  > 2$
5	PE4	D	507	-	13,13,23	0.19	0	12,12,22	0.17	0
4	GOL	D	505	-	5,5,5	0.08	0	5,5,5	0.29	0
4	GOL	A	505	-	5,5,5	0.90	0	5,5,5	0.99	0
4	GOL	A	504	-	5,5,5	0.89	0	5,5,5	0.99	0
4	GOL	D	506	-	5,5,5	0.89	0	5,5,5	1.01	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
5	PE4	D	507	-	-	4/11/11/21	-
4	GOL	D	505	-	-	1/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	D	506	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

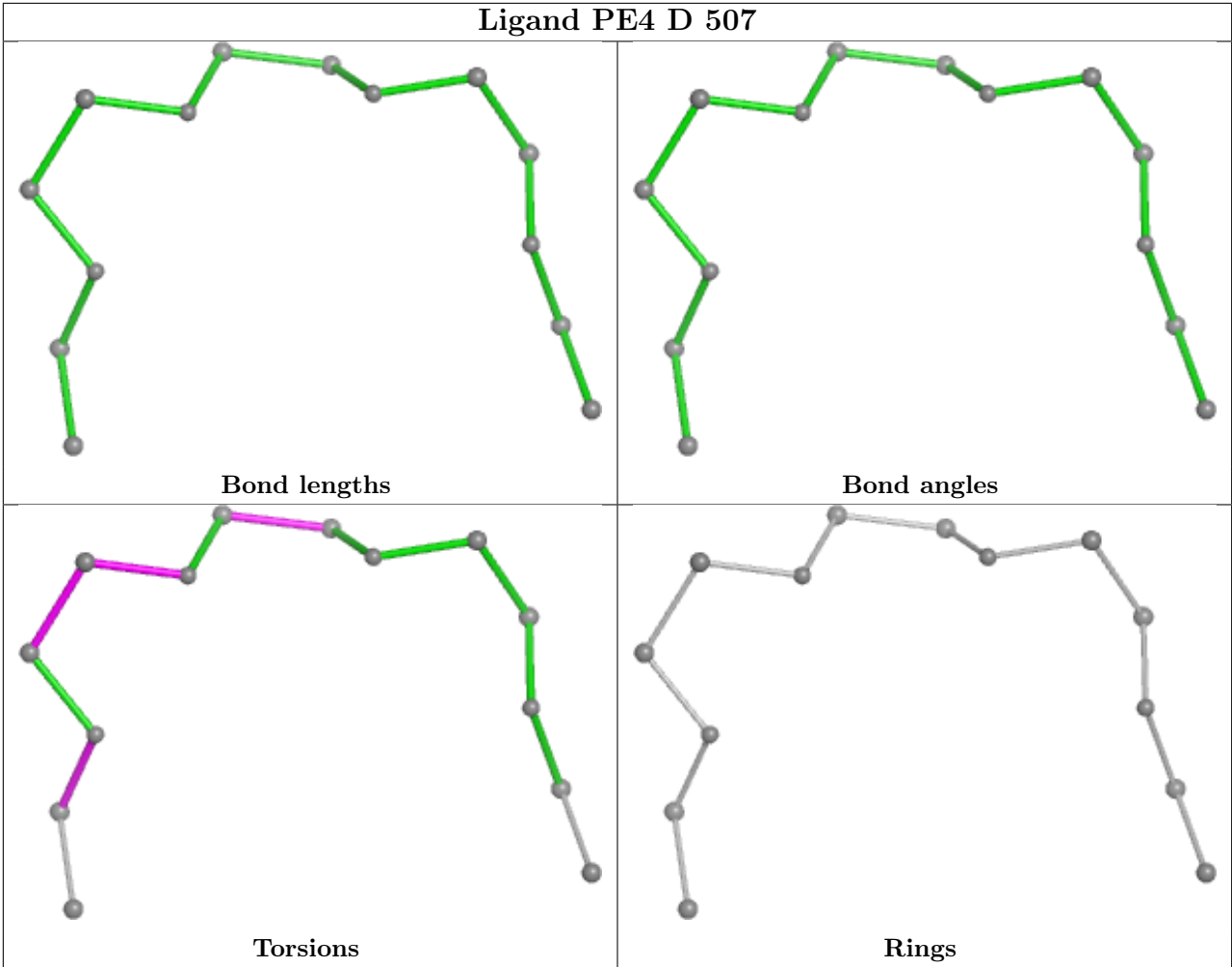
Mol	Chain	Res	Type	Atoms
4	D	505	GOL	C1-C2-C3-O3
5	D	507	PE4	O2-C3-C4-O3
5	D	507	PE4	O3-C5-C6-O4
5	D	507	PE4	C1-C2-O2-C3
5	D	507	PE4	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	507	PE4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	145[A]:ASN	C	146:ARG	N	1.12
1	D	145[B]:ASN	C	146:ARG	N	1.07



## 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	417/422 (98%)	0.59	22 (5%)	33 30	34, 66, 99, 126	2 (0%)
1	D	417/422 (98%)	0.49	36 (8%)	18 16	29, 61, 99, 122	2 (0%)
2	B	6/24 (25%)	1.44	2 (33%)	1 1	58, 61, 83, 93	0
2	E	6/24 (25%)	1.44	3 (50%)	0 0	76, 79, 93, 129	0
All	All	846/892 (94%)	0.55	63 (7%)	22 20	29, 65, 99, 129	4 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	LEU	6.1
1	D	36	VAL	5.1
1	A	6	ASP	5.0
1	A	204	LEU	4.7
1	D	35	TYR	3.9
1	A	39	ASP	3.9
1	A	35	TYR	3.9
1	A	205	GLY	3.8
1	D	131	THR	3.7
1	D	88	ALA	3.6
1	D	20	PRO	3.5
1	A	104	GLY	3.4
2	B	201	GLN	3.4
1	A	36	VAL	3.3
1	A	7	TYR	3.3
1	A	206	THR	3.2
1	A	203	GLY	3.1
1	D	48	LYS	3.0
2	E	206	VAL	3.0
1	A	99	ARG	3.0
1	A	200	SER	3.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	9	VAL	2.8
1	D	161	ARG	2.8
1	D	203	GLY	2.7
1	D	100	LEU	2.7
1	A	49	GLU	2.6
1	A	133	GLY	2.6
1	D	39	ASP	2.6
1	D	265[A]	ASP	2.6
1	D	19	GLY	2.6
1	D	37	SER	2.6
1	D	103	GLN	2.6
1	A	283	ASP	2.6
2	E	201	GLN	2.6
1	D	77	LEU	2.5
1	D	55	LEU	2.5
1	D	49	GLU	2.5
1	D	266	GLY	2.5
1	D	123	LEU	2.4
1	D	91	ALA	2.4
1	D	41	GLY	2.4
1	D	102	VAL	2.4
1	D	112	ALA	2.4
1	D	6	ASP	2.4
1	A	88	ALA	2.4
2	B	202	SER	2.4
1	D	46	ARG	2.3
1	D	205	GLY	2.3
1	A	101	GLN	2.3
1	D	38	ASN	2.2
1	D	7	TYR	2.2
1	A	114	THR	2.2
1	D	160	ARG	2.2
2	E	202	SER	2.2
1	A	201	MET	2.1
1	A	131	THR	2.1
1	D	21	SER	2.1
1	D	162	THR	2.1
1	D	164	LYS	2.1
1	D	101	GLN	2.1
1	A	163	LYS	2.1
1	D	29	GLY	2.0
1	D	120	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

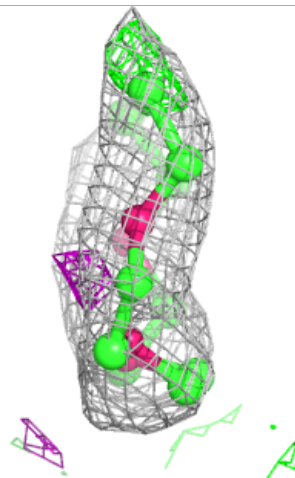
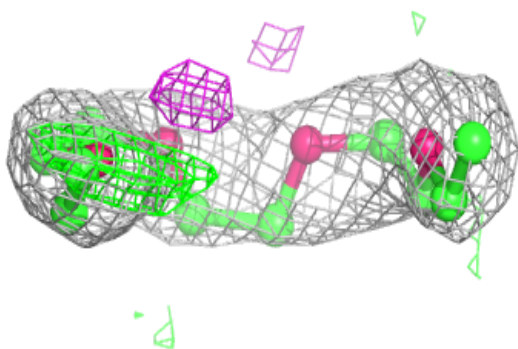
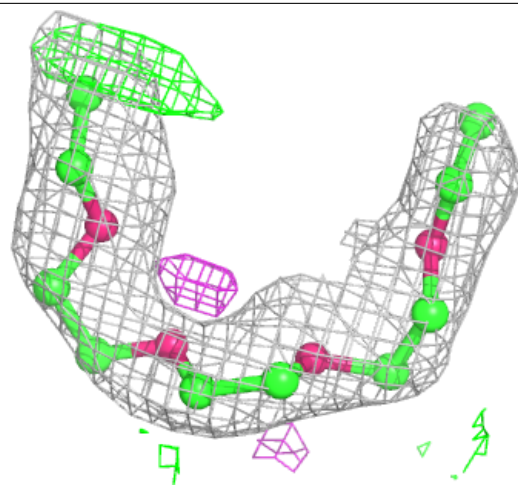
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	D	502	1/1	0.55	0.18	126,126,126,126	0
3	CA	D	501	1/1	0.61	0.15	120,120,120,120	0
3	CA	A	506	1/1	0.65	0.15	142,142,142,142	0
3	CA	D	508	1/1	0.70	0.16	123,123,123,123	0
3	CA	A	501	1/1	0.75	0.10	103,103,103,103	0
5	PE4	D	507	14/24	0.81	0.22	72,85,88,88	0
4	GOL	D	505	6/6	0.90	0.14	55,57,60,62	0
3	CA	D	504	1/1	0.92	0.09	53,53,53,53	0
3	CA	A	502	1/1	0.93	0.06	91,91,91,91	0
4	GOL	A	505	6/6	0.94	0.09	53,56,56,57	0
4	GOL	D	506	6/6	0.94	0.09	38,39,40,41	0
4	GOL	A	504	6/6	0.95	0.10	70,70,70,71	0
3	CA	A	503	1/1	0.97	0.06	66,66,66,66	0
3	CA	D	503	1/1	0.99	0.04	65,65,65,65	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 PE4 D 507:**

$2mF_o-DF_c$  (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.