



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:53 am BST

PDB ID : 3NFI
Title : Crystal structure of tandem winged helix domain of RNA polymerase I subunit A49
Authors : Geiger, S.R.; Lorenzen, K.; Schrieck, A.; Hanecker, P.; Kostrewa, D.; Heck, A.J.R.; Cramer, P.
Deposited on : 2010-06-10
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

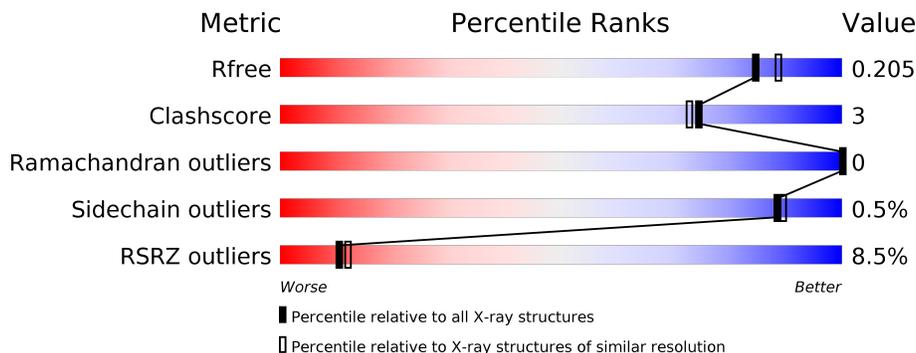
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	237	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	B	237	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	C	237	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div>
1	D	237	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
1	E	237	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9695 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 DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	219	Total 1798	C 1167	N 296	O 329	S 1	Se 5	0	9	0
1	B	227	Total 1838	C 1189	N 304	O 338	S 1	Se 6	0	5	0
1	C	214	Total 1750	C 1139	N 285	O 319	S 1	Se 6	0	9	0
1	D	220	Total 1790	C 1161	N 296	O 327	S 1	Se 5	0	6	0
1	E	212	Total 1721	C 1120	N 278	O 316	S 1	Se 6	0	7	0

There are 30 discrepancies between the modelled and reference sequences:

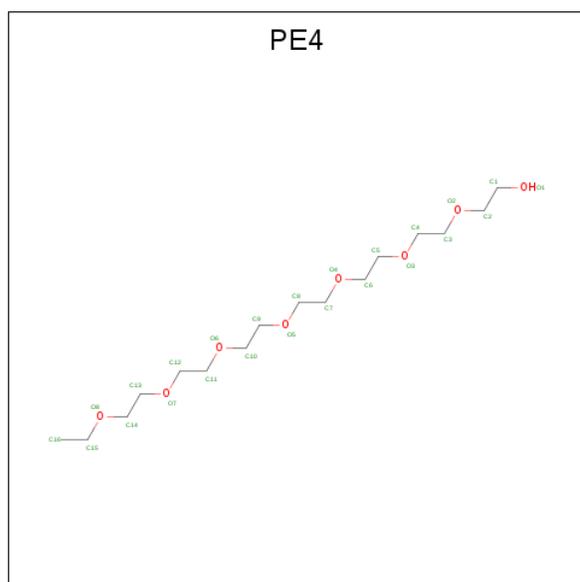
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	GLY	-	EXPRESSION TAG	UNP Q01080
A	168	SER	-	EXPRESSION TAG	UNP Q01080
A	169	HIS	-	EXPRESSION TAG	UNP Q01080
A	170	MSE	-	EXPRESSION TAG	UNP Q01080
A	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
A	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
B	167	GLY	-	EXPRESSION TAG	UNP Q01080
B	168	SER	-	EXPRESSION TAG	UNP Q01080
B	169	HIS	-	EXPRESSION TAG	UNP Q01080
B	170	MSE	-	EXPRESSION TAG	UNP Q01080
B	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
B	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
C	167	GLY	-	EXPRESSION TAG	UNP Q01080
C	168	SER	-	EXPRESSION TAG	UNP Q01080
C	169	HIS	-	EXPRESSION TAG	UNP Q01080
C	170	MSE	-	EXPRESSION TAG	UNP Q01080
C	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
C	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
D	167	GLY	-	EXPRESSION TAG	UNP Q01080

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Chain	Residue	Modelled	Actual	Comment	Reference
D	168	SER	-	EXPRESSION TAG	UNP Q01080
D	169	HIS	-	EXPRESSION TAG	UNP Q01080
D	170	MSE	-	EXPRESSION TAG	UNP Q01080
D	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
D	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
E	167	GLY	-	EXPRESSION TAG	UNP Q01080
E	168	SER	-	EXPRESSION TAG	UNP Q01080
E	169	HIS	-	EXPRESSION TAG	UNP Q01080
E	170	MSE	-	EXPRESSION TAG	UNP Q01080
E	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
E	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080

- Molecule 2 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total	0	0
			C		
			12	8	4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	226	Total	0	0
			O		
			226	226	
3	B	146	Total	0	0
			O		
			146	146	

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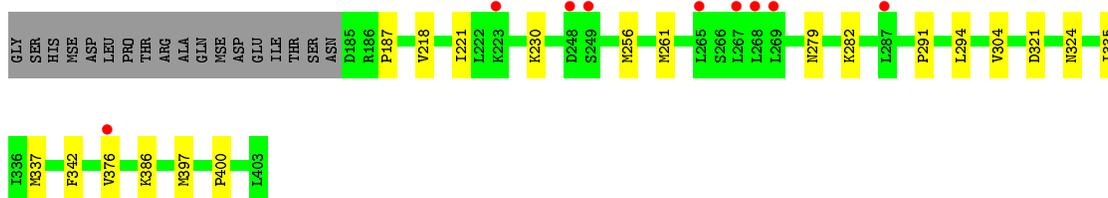
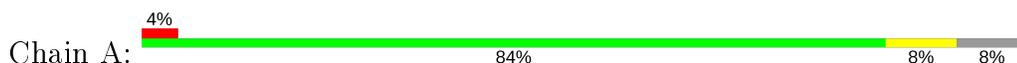
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	116	Total 116	O 116	0	0
3	D	156	Total 156	O 156	0	0
3	E	142	Total 142	O 142	0	0

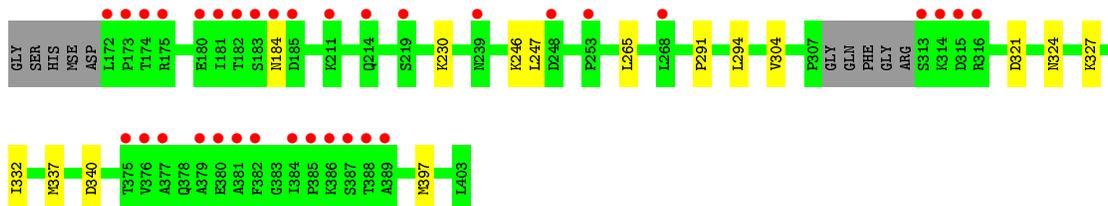
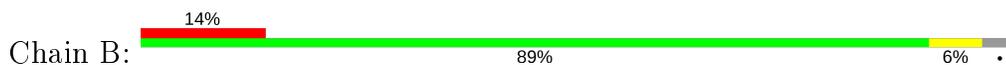
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

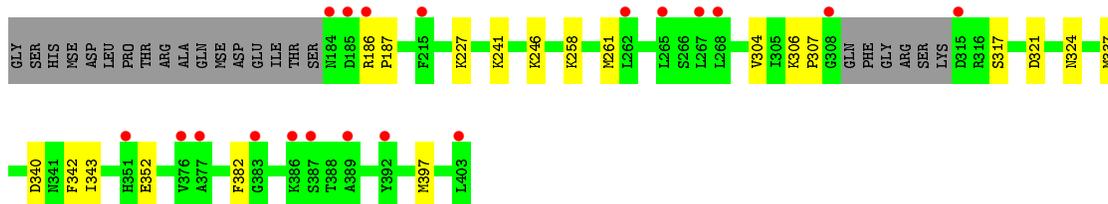
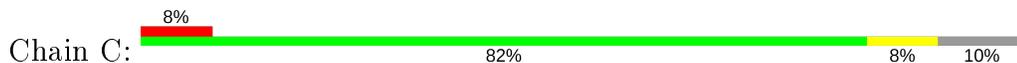
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



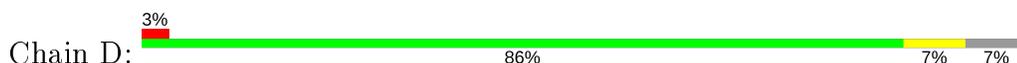
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49

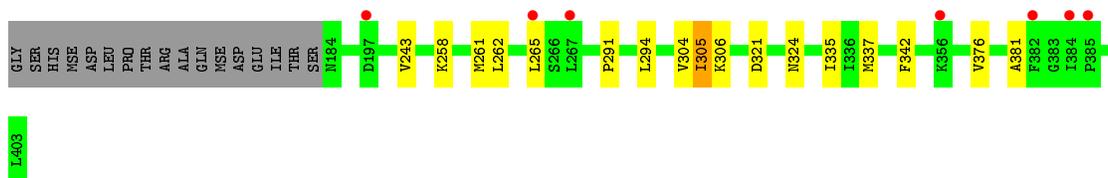


- Molecule 1: DNA-directed RNA polymerase I subunit RPA49

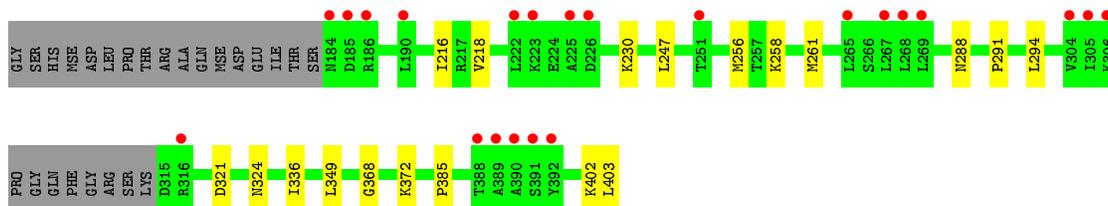
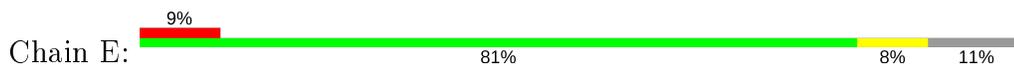


- Molecule 1: DNA-directed RNA polymerase I subunit RPA49





- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.11Å 78.10Å 100.67Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	27.82 – 1.90 30.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.82-1.90) 98.3 (30.87-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.89Å)	Xtrriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.189 , 0.224 0.203 , 0.205	Depositor DCC
R_{free} test set	4564 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9695	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: PE4

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	0.50	0/1852	0.61	0/2496
1	B	0.46	0/1878	0.59	0/2531
1	C	0.47	0/1805	0.62	0/2433
1	D	0.51	0/1834	0.62	0/2471
1	E	0.64	1/1768 (0.1%)	0.60	0/2383
All	All	0.52	1/9137 (0.0%)	0.61	0/12314

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	403	LEU	C-OXT	-15.93	0.93	1.23

There are no bond angle outliers.

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	1798	0	1902	15	0
1	B	1838	0	1936	11	0
1	C	1750	0	1861	13	0
1	D	1790	0	1890	9	0
1	E	1721	0	1817	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	12	0	14	1	0
3	A	226	0	0	1	0
3	B	146	0	0	0	0
3	C	116	0	0	0	0
3	D	156	0	0	0	0
3	E	142	0	0	1	0
All	All	9695	0	9420	58	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 3.

All (58) 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:218:VAL:HG23	1:A:256:MSE:SE	2.30	0.80
1:A:337[B]:MSE:SE	1:A:397:MSE:HG3	2.32	0.79
1:C:337[B]:MSE:SE	1:C:397:MSE:SE	3.03	0.77
1:A:187:PRO:HB2	3:A:781:HOH:O	1.85	0.77
1:C:337[B]:MSE:SE	1:C:397:MSE:HG3	2.36	0.76
1:B:184:ASN:HA	1:B:327:LYS:HZ2	1.51	0.75
1:A:337[B]:MSE:SE	1:A:397:MSE:SE	3.05	0.74
1:B:184:ASN:HA	1:B:327:LYS:NZ	2.04	0.72
1:A:304:VAL:HG23	1:A:324:ASN:HD21	1.55	0.70
1:B:304:VAL:HG23	1:B:324:ASN:HD21	1.55	0.70
1:E:218:VAL:HG23	1:E:256[B]:MSE:SE	2.47	0.65
1:B:337[B]:MSE:SE	1:B:397:MSE:SE	3.16	0.63
1:D:304:VAL:HG23	1:D:324:ASN:HD21	1.64	0.62
1:C:304:VAL:HG23	1:C:324:ASN:HD21	1.67	0.60
1:A:337[B]:MSE:SE	1:A:397:MSE:CG	2.99	0.60
1:E:372:LYS:HA	2:E:1:PE4:H121	1.82	0.60
1:E:368:GLY:CA	1:E:402:LYS:HE3	2.32	0.59
1:C:241:LYS:HB2	1:C:352:GLU:OE1	2.03	0.58
1:E:368:GLY:HA2	1:E:402:LYS:HE3	1.84	0.58
1:C:337[B]:MSE:SE	1:C:397:MSE:CG	3.01	0.58
1:A:321:ASP:H	1:A:324:ASN:HD22	1.53	0.55
1:A:218:VAL:CG2	1:A:256:MSE:SE	3.02	0.55
1:D:321:ASP:H	1:D:324:ASN:HD22	1.54	0.54
1:B:321:ASP:H	1:B:324:ASN:HD22	1.55	0.54
1:E:321:ASP:H	1:E:324:ASN:HD22	1.56	0.53
1:A:400:PRO:HB3	1:C:307:PRO:HB2	1.90	0.52
1:A:221:ILE:HG23	1:A:230:LYS:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MSE:HB3	1:A:335:ILE:HG23	1.94	0.50
1:D:305:ILE:HG12	1:D:306:LYS:N	2.27	0.49
1:B:265[B]:LEU:HD11	1:B:332:ILE:HG23	1.96	0.47
1:C:343:ILE:HG12	1:C:382:PHE:HZ	1.79	0.47
1:D:337:MSE:SE	1:D:342:PHE:HA	2.65	0.47
1:A:337[A]:MSE:SE	1:A:342:PHE:HA	2.65	0.46
1:C:337[A]:MSE:SE	1:C:342:PHE:HA	2.65	0.46
1:D:381:ALA:HA	1:E:385:PRO:HB3	1.98	0.45
1:D:265:LEU:HB2	1:D:335:ILE:HG21	1.98	0.45
1:E:288:ASN:ND2	3:E:503:HOH:O	2.50	0.45
1:B:246:LYS:HE3	1:B:340:ASP:OD1	2.17	0.45
1:D:291:PRO:HD2	1:D:294:LEU:HD12	1.98	0.45
1:E:336:ILE:HD13	1:E:349:LEU:HD11	1.99	0.44
1:D:243:VAL:HA	1:D:262:LEU:HD11	1.99	0.44
1:B:265[B]:LEU:CD1	1:B:332:ILE:HG23	2.47	0.44
1:C:246:LYS:HE3	1:C:340:ASP:OD1	2.18	0.44
1:C:186:ARG:HG3	1:C:187:PRO:HD2	1.99	0.44
1:A:291:PRO:HD2	1:A:294:LEU:HD12	2.00	0.44
1:C:306:LYS:HG3	1:C:317:SER:HB3	1.99	0.43
1:C:258:LYS:HA	1:C:261:MSE:HE3	2.00	0.43
1:E:216:ILE:HG12	1:E:294:LEU:HD11	2.01	0.43
1:E:230:LYS:HB3	1:E:247:LEU:HD21	2.01	0.43
1:B:230:LYS:HB3	1:B:247:LEU:HD21	2.01	0.42
1:C:321:ASP:H	1:C:324:ASN:HD22	1.67	0.42
1:A:337[B]:MSE:CE	1:A:397:MSE:HG3	2.49	0.42
1:D:258:LYS:HA	1:D:261:MSE:HE3	2.02	0.41
1:A:279:ASN:HD21	1:A:282:LYS:HD2	1.85	0.41
1:B:291:PRO:HD2	1:B:294:LEU:HD12	2.02	0.41
1:E:291:PRO:HD2	1:E:294:LEU:HD12	2.02	0.41
1:E:258:LYS:HA	1:E:261:MSE:HE3	2.02	0.40
1:B:337[B]:MSE:SE	1:B:397:MSE:HG3	2.72	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	226/237 (95%)	221 (98%)	5 (2%)	0	100	100
1	B	228/237 (96%)	227 (100%)	1 (0%)	0	100	100
1	C	219/237 (92%)	217 (99%)	2 (1%)	0	100	100
1	D	224/237 (94%)	219 (98%)	5 (2%)	0	100	100
1	E	215/237 (91%)	213 (99%)	2 (1%)	0	100	100
All	All	1112/1185 (94%)	1097 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	207/208 (100%)	205 (99%)	2 (1%)	76	76
1	B	211/208 (101%)	211 (100%)	0	100	100
1	C	203/208 (98%)	202 (100%)	1 (0%)	88	89
1	D	205/208 (99%)	203 (99%)	2 (1%)	76	76
1	E	197/208 (95%)	197 (100%)	0	100	100
All	All	1023/1040 (98%)	1018 (100%)	5 (0%)	88	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	VAL
1	A	386	LYS
1	C	227	LYS
1	D	305	ILE
1	D	376	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	278	ASN
1	A	324	ASN
1	B	237	GLN
1	B	324	ASN
1	B	341	ASN
1	C	238	ASN
1	C	252	GLN
1	C	324	ASN
1	D	324	ASN
1	D	341	ASN
1	E	252	GLN
1	E	324	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PE4	E	1	-	11,11,23	1.05	0	10,10,22	1.80	3 (30%)

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	PE4	E	1	-	-	1/9/9/21	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	PE4	O7-C12-C11	2.97	123.81	110.39
2	E	1	PE4	O5-C8-C7	-2.64	98.48	110.07
2	E	1	PE4	C11-O6-C10	2.49	124.07	113.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	PE4	O6-C11-C12-O7

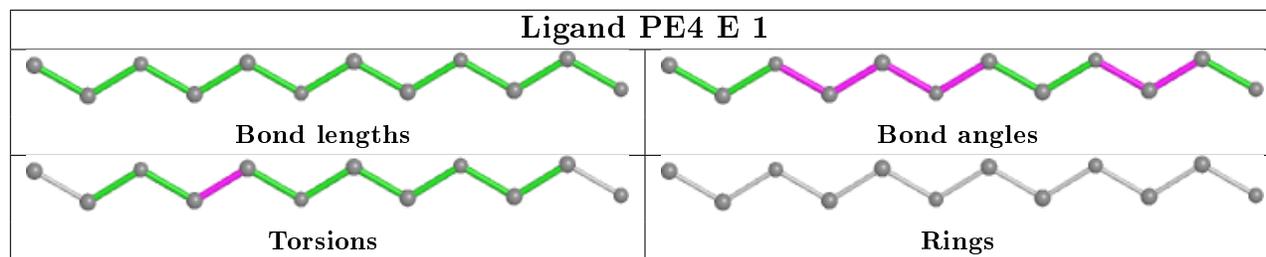
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	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 [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	215/237 (90%)	0.05	9 (4%) 36 39	21, 31, 58, 79	0
1	B	222/237 (93%)	0.68	34 (15%) 2 2	22, 40, 100, 131	0
1	C	210/237 (88%)	0.30	19 (9%) 9 10	24, 40, 70, 100	0
1	D	216/237 (91%)	0.02	7 (3%) 47 50	18, 31, 59, 84	0
1	E	208/237 (87%)	0.27	22 (10%) 6 7	22, 34, 65, 103	0
All	All	1071/1185 (90%)	0.27	91 (8%) 10 12	18, 35, 75, 131	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	THR	10.0
1	B	314	LYS	8.3
1	B	313	SER	7.3
1	E	184	ASN	6.4
1	B	315	ASP	6.3
1	B	182	THR	5.5
1	B	386	LYS	5.4
1	E	185	ASP	5.3
1	B	384	ILE	5.1
1	B	253	PRO	5.1
1	B	376	VAL	4.7
1	E	305	ILE	4.6
1	C	389	ALA	4.6
1	C	392	TYR	4.3
1	C	387	SER	4.0
1	B	183	SER	4.0
1	C	308	GLY	3.9
1	B	175	ARG	3.9
1	B	173	PRO	3.8
1	B	316	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	316	ARG	3.6
1	E	225	ALA	3.5
1	E	388	THR	3.5
1	C	376	VAL	3.4
1	D	384	ILE	3.4
1	C	351[A]	HIS	3.4
1	B	219	SER	3.3
1	C	268	LEU	3.3
1	C	185	ASP	3.3
1	B	214	GLN	3.1
1	B	379	ALA	3.0
1	B	385	PRO	3.0
1	B	180	GLU	3.0
1	E	222	LEU	2.9
1	E	269	LEU	2.9
1	E	251	THR	2.9
1	B	381	ALA	2.9
1	B	380	GLU	2.8
1	E	392	TYR	2.8
1	A	267	LEU	2.8
1	B	375	THR	2.8
1	E	389	ALA	2.8
1	A	268	LEU	2.8
1	E	226	ASP	2.7
1	C	265[A]	LEU	2.7
1	B	181	ILE	2.7
1	B	211	LYS	2.7
1	B	248	ASP	2.7
1	B	185	ASP	2.6
1	B	184	ASN	2.6
1	B	239	ASN	2.6
1	E	306	LYS	2.6
1	B	172	LEU	2.6
1	D	197[A]	ASP	2.6
1	C	184	ASN	2.5
1	E	265	LEU	2.5
1	C	215	PHE	2.5
1	B	377	ALA	2.5
1	A	376	VAL	2.5
1	D	356	LYS	2.5
1	C	267	LEU	2.5
1	E	304	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	186	ARG	2.4
1	D	267	LEU	2.4
1	E	267	LEU	2.4
1	C	383	GLY	2.4
1	B	388	THR	2.4
1	C	386	LYS	2.4
1	A	265	LEU	2.3
1	A	287	LEU	2.3
1	A	223	LYS	2.3
1	A	248	ASP	2.3
1	C	377	ALA	2.2
1	A	269	LEU	2.2
1	C	315	ASP	2.2
1	A	249	SER	2.2
1	B	387	SER	2.2
1	B	389	ALA	2.2
1	D	385	PRO	2.1
1	C	403	LEU	2.1
1	D	265	LEU	2.1
1	C	262	LEU	2.1
1	D	382	PHE	2.1
1	E	390	ALA	2.1
1	E	186	ARG	2.0
1	E	268	LEU	2.0
1	B	382	PHE	2.0
1	B	268	LEU	2.0
1	E	190	LEU	2.0
1	E	223	LYS	2.0
1	E	391	SER	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](#)

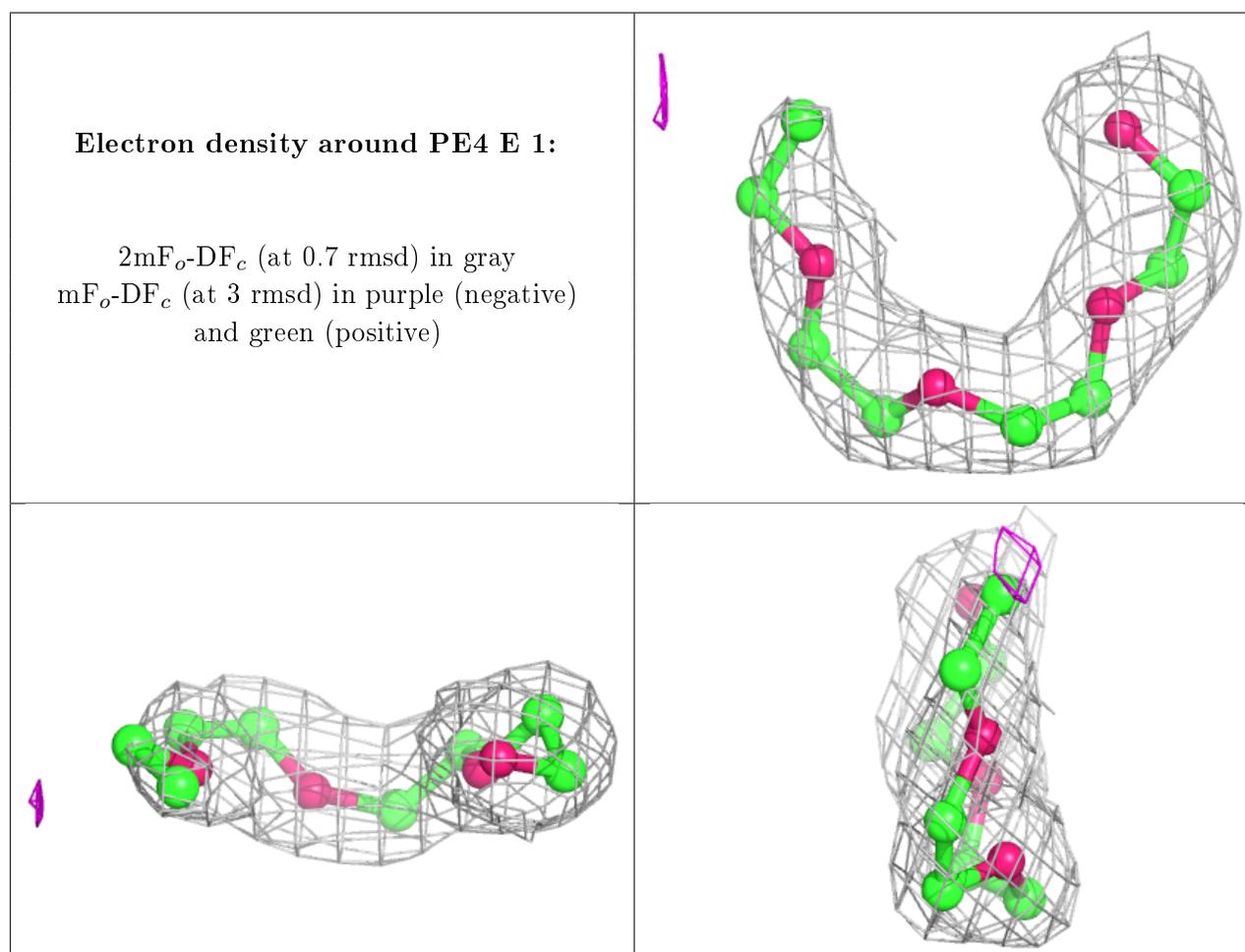
There are no carbohydrates in this entry.

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
2	PE4	E	1	12/24	0.94	0.17	32,36,47,47	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.