



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:57 pm BST

PDB ID : 3P7Z
Title : Crystal structure of the Neurofibromin Sec14-PH module containing the patient derived mutation I1584V
Authors : Welti, S.; Scheffzek, K.
Deposited on : 2010-10-13
Resolution : 2.65 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

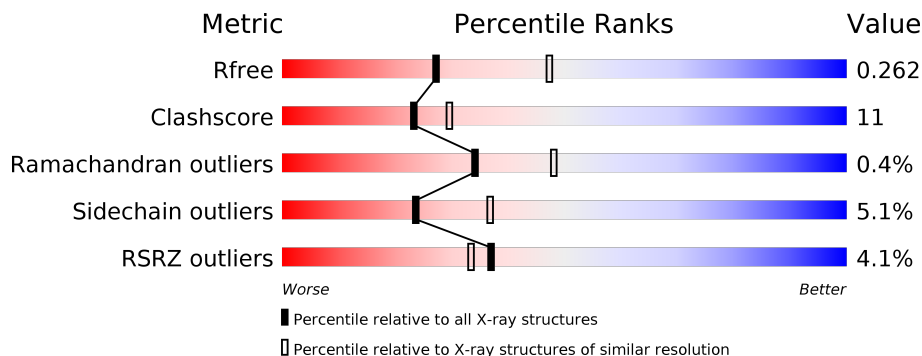
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	276	
1	B	276	

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
2	PEV	A	1	X	-	-	-
2	PEV	B	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4659 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.

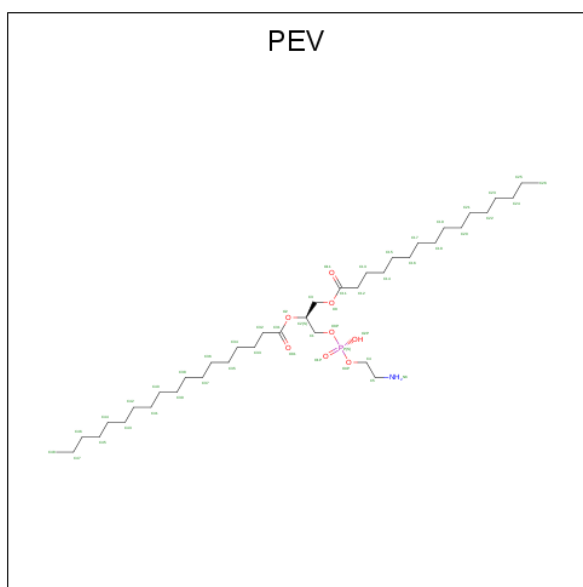
- Molecule 1 is a protein called Neurofibromin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2182	1410	365	401	6	0	0	0
1	B	270	2194	1418	367	403	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1541	GLY	-	EXPRESSION TAG	UNP P21359
A	1542	ALA	-	EXPRESSION TAG	UNP P21359
A	1543	MET	-	EXPRESSION TAG	UNP P21359
A	1544	GLY	-	EXPRESSION TAG	UNP P21359
A	1584	VAL	ILE	ENGINEERED MUTATION	UNP P21359
B	1541	GLY	-	EXPRESSION TAG	UNP P21359
B	1542	ALA	-	EXPRESSION TAG	UNP P21359
B	1543	MET	-	EXPRESSION TAG	UNP P21359
B	1544	GLY	-	EXPRESSION TAG	UNP P21359
B	1584	VAL	ILE	ENGINEERED MUTATION	UNP P21359

- Molecule 2 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P).

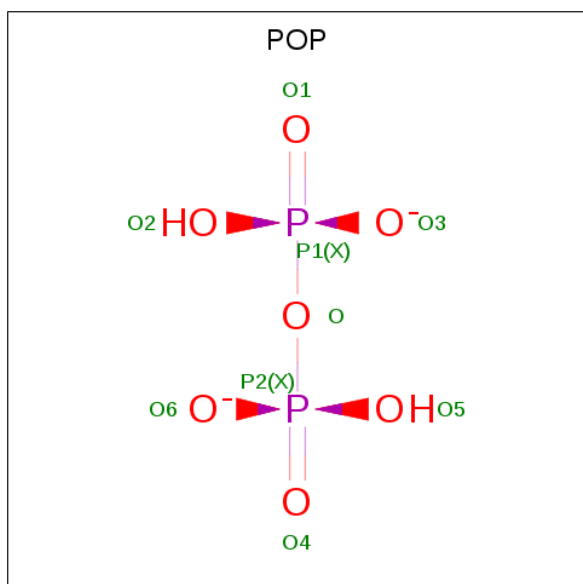


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	49	39	1	8	1	3	0
2	B	1	49	39	1	8	1	3	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		

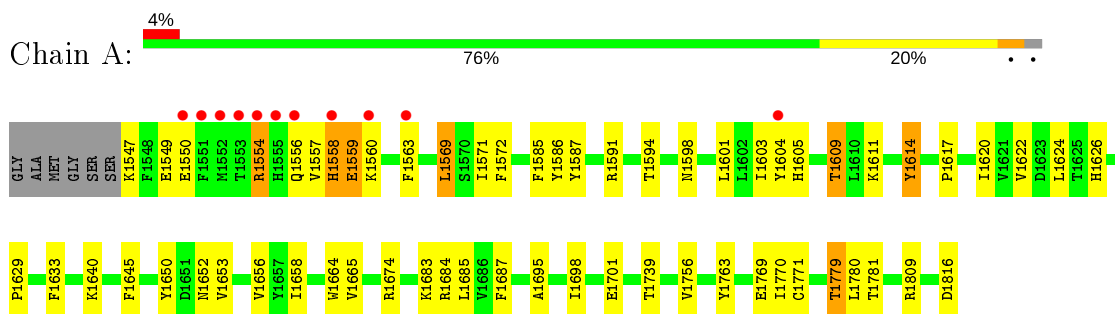
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	103	Total	O	0	0
			103	103		

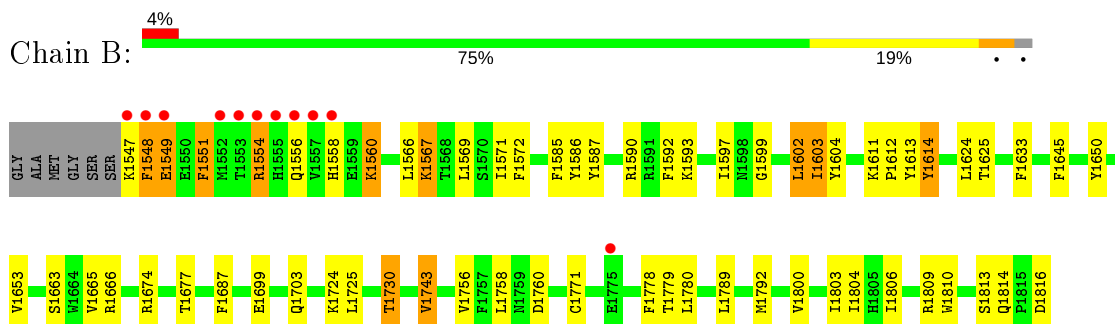
3 Residue-property plots [i](#)

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: Neurofibromin



- Molecule 1: Neurofibromin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.06Å 113.06Å 124.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.65 49.14 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.00-2.65) 100.0 (49.14-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.65Å)	Xtrriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.216 , 0.266 0.213 , 0.262	Depositor DCC
R_{free} test set	1229 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4659	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: NA, PEV, POP

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	0.22	0/2237	0.38	0/3035
1	B	0.21	0/2249	0.38	0/3048
All	All	0.21	0/4486	0.38	0/6083

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	2182	0	2143	45	0
1	B	2194	0	2169	46	0
2	A	49	0	77	8	0
2	B	49	0	77	9	0
3	A	1	0	0	0	0
4	B	18	0	0	0	0
5	A	63	0	0	0	0
5	B	103	0	0	0	0
All	All	4659	0	4466	101	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 11.

All (101) 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:B:1674:ARG:HH11	1:B:1674:ARG:HG3	1.44	0.83
1:A:1569:LEU:HD13	1:A:1571:ILE:HG13	1.64	0.79
1:A:1571:ILE:HG12	1:A:1591:ARG:HB3	1.67	0.76
1:B:1743:VAL:HG13	1:B:1760:ASP:HB2	1.69	0.73
1:B:1806:ILE:HA	1:B:1809:ARG:HG2	1.72	0.71
1:A:1645:PHE:HB2	1:A:1650:TYR:CZ	2.27	0.70
1:A:1559:GLU:HB2	1:A:1563:PHE:CD1	2.26	0.70
1:A:1653:VAL:HG21	2:A:1:PEV:H32	1.75	0.68
1:B:1611:LYS:HB3	1:B:1612:PRO:HD3	1.76	0.67
1:B:1645:PHE:HB2	1:B:1650:TYR:CZ	2.30	0.67
1:B:1547:LYS:HD2	1:B:1549:GLU:HG3	1.76	0.66
1:B:1548:PHE:HA	1:B:1551:PHE:HB2	1.79	0.65
1:B:1554:ARG:HG2	1:B:1604:TYR:CG	2.32	0.65
1:A:1550:GLU:O	1:A:1554:ARG:HB2	1.97	0.64
2:A:1:PEV:H441	2:A:1:PEV:H351	1.79	0.64
2:B:1:PEV:H382	2:B:1:PEV:H421	1.78	0.64
1:A:1769:GLU:HB2	1:A:1781:THR:HB	1.80	0.63
1:B:1724:LYS:HB3	1:B:1730:THR:HG23	1.81	0.62
1:A:1547:LYS:HE3	1:A:1549:GLU:HB2	1.82	0.62
1:A:1554:ARG:HG3	1:A:1604:TYR:CG	2.35	0.62
2:A:1:PEV:H462	2:A:1:PEV:H332	1.82	0.61
1:B:1725:LEU:HD21	1:B:1792:MET:HG3	1.83	0.60
1:B:1653:VAL:HG11	2:B:1:PEV:H321	1.82	0.60
1:A:1687:PHE:CG	1:A:1756:VAL:HG11	2.37	0.59
1:B:1674:ARG:HG3	1:B:1674:ARG:NH1	2.14	0.59
1:A:1656:VAL:HG21	2:A:1:PEV:H321	1.84	0.58
2:B:1:PEV:H121	2:B:1:PEV:H332	1.86	0.57
1:B:1653:VAL:HG21	2:B:1:PEV:H322	1.88	0.56
1:A:1611:LYS:HA	1:A:1614:TYR:CZ	2.41	0.55
1:A:1572:PHE:HA	1:A:1586:TYR:O	2.07	0.54
1:B:1548:PHE:HA	1:B:1551:PHE:CB	2.37	0.54
1:A:1653:VAL:HB	1:A:1684:ARG:NH2	2.22	0.53
1:A:1770:ILE:H	1:A:1770:ILE:HD12	1.73	0.53
1:B:1569:LEU:HD11	1:B:1571:ILE:HB	1.91	0.52
1:B:1687:PHE:CG	1:B:1756:VAL:HG11	2.45	0.52
1:B:1624:LEU:HD13	1:B:1665:VAL:HG11	1.93	0.51
1:B:1566:LEU:HD23	1:B:1569:LEU:HD21	1.93	0.50
1:A:1605:HIS:O	1:A:1609:THR:HG22	2.10	0.50
1:B:1803:ILE:O	1:B:1806:ILE:HG12	2.11	0.50
1:A:1624:LEU:HD13	1:A:1665:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1622:VAL:HG13	1:A:1658:ILE:HA	1.95	0.49
1:A:1695:ALA:HA	1:A:1698:ILE:O	2.12	0.49
1:B:1810:TRP:O	1:B:1814:GLN:HG2	2.13	0.48
1:B:1593:LYS:H	1:B:1597:ILE:HD12	1.79	0.47
1:B:1699:GLU:O	1:B:1703:GLN:HG3	2.14	0.47
1:A:1701:GLU:CD	1:A:1701:GLU:H	2.16	0.47
1:B:1567:LYS:HE3	1:B:1567:LYS:HA	1.96	0.47
1:A:1603:ILE:HD12	1:A:1640:LYS:HD2	1.97	0.47
1:A:1554:ARG:HG3	1:A:1604:TYR:CD1	2.50	0.47
1:B:1572:PHE:HA	1:B:1586:TYR:O	2.14	0.47
2:A:1:PEV:H432	2:A:1:PEV:H191	1.96	0.46
1:A:1771:CYS:HB3	1:A:1779:THR:HB	1.98	0.46
1:B:1599:GLY:O	1:B:1603:ILE:HG22	2.16	0.46
2:B:1:PEV:H241	2:B:1:PEV:C3	2.46	0.46
1:B:1585:PHE:HZ	1:B:1613:TYR:CG	2.34	0.45
1:B:1560:LYS:NZ	1:B:1560:LYS:HB3	2.32	0.45
1:B:1590:ARG:NH1	1:B:1625:THR:HB	2.31	0.45
2:B:1:PEV:H161	2:B:1:PEV:H191	1.86	0.45
1:B:1592:PHE:CD2	1:B:1602:LEU:HD12	2.51	0.45
1:A:1629:PRO:HA	1:A:1664:TRP:CZ2	2.52	0.45
1:A:1629:PRO:HG3	1:A:1664:TRP:NE1	2.33	0.44
1:A:1739:THR:HG21	1:B:1813:SER:HB3	1.98	0.44
1:B:1554:ARG:HG2	1:B:1604:TYR:CD1	2.52	0.44
1:B:1592:PHE:HA	1:B:1597:ILE:HD12	1.98	0.44
1:B:1699:GLU:OE2	1:B:1699:GLU:HA	2.17	0.44
1:A:1611:LYS:HA	1:A:1614:TYR:CE1	2.52	0.44
1:A:1598:ASN:HB3	1:A:1601:LEU:HD12	1.99	0.44
2:B:1:PEV:H342	2:B:1:PEV:H31	2.00	0.44
1:A:1556:GLN:CD	1:A:1557:VAL:HG23	2.38	0.44
1:A:1633:PHE:CE1	2:A:1:PEV:H222	2.53	0.44
2:A:1:PEV:H152	2:A:1:PEV:H121	1.87	0.43
1:A:1683:LYS:HD2	1:A:1683:LYS:HA	1.61	0.43
1:B:1569:LEU:CD1	1:B:1571:ILE:HB	2.48	0.43
1:B:1666:ARG:HD2	1:B:1758:LEU:HD11	2.01	0.43
1:A:1554:ARG:HD3	1:A:1554:ARG:HA	1.59	0.43
1:A:1563:PHE:HB2	1:A:1601:LEU:HD22	2.00	0.43
1:A:1587:TYR:HH	1:A:1633:PHE:HZ	1.63	0.43
2:B:1:PEV:H241	2:B:1:PEV:H32	2.01	0.43
1:A:1556:GLN:NE2	1:A:1557:VAL:HG23	2.34	0.43
1:A:1653:VAL:HB	1:A:1684:ARG:HH21	1.83	0.42
1:B:1725:LEU:N	1:B:1725:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1778:PHE:HE1	1:B:1780:LEU:HG	1.84	0.42
1:A:1585:PHE:HB2	1:A:1620:ILE:CD1	2.49	0.41
1:B:1587:TYR:HH	1:B:1633:PHE:HZ	1.66	0.41
1:B:1779:THR:HA	1:B:1789:LEU:O	2.20	0.41
1:B:1614:TYR:C	1:B:1614:TYR:CD1	2.94	0.41
1:B:1771:CYS:HB2	1:B:1779:THR:OG1	2.20	0.41
1:A:1617:PRO:HA	1:A:1652:ASN:O	2.20	0.41
2:A:1:PEV:H52	2:A:1:PEV:O2P	2.21	0.41
1:A:1559:GLU:O	1:A:1559:GLU:HG2	2.20	0.41
1:A:1560:LYS:HZ3	1:A:1560:LYS:HB3	1.85	0.41
1:A:1809:ARG:HA	1:A:1809:ARG:HD2	1.95	0.41
2:B:1:PEV:H172	2:B:1:PEV:H142	1.79	0.41
1:B:1663:SER:HA	1:B:1758:LEU:HD13	2.03	0.41
1:B:1674:ARG:O	1:B:1677:THR:HG23	2.21	0.40
1:B:1614:TYR:HD1	1:B:1614:TYR:C	2.23	0.40
1:A:1770:ILE:N	1:A:1770:ILE:HD12	2.37	0.40
1:A:1816:ASP:OD2	1:B:1590:ARG:HB2	2.21	0.40
1:A:1560:LYS:HB3	1:A:1560:LYS:NZ	2.35	0.40
1:A:1626:HIS:CE1	1:A:1763:TYR:CE1	3.10	0.40
1:B:1800:VAL:O	1:B:1804:ILE:HG13	2.21	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	268/276 (97%)	254 (95%)	13 (5%)	1 (0%)	34 48
1	B	268/276 (97%)	252 (94%)	15 (6%)	1 (0%)	34 48
All	All	536/552 (97%)	506 (94%)	28 (5%)	2 (0%)	34 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1558	HIS
1	B	1560	LYS

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	235/243 (97%)	224 (95%)	11 (5%)	26	40
1	B	238/243 (98%)	225 (94%)	13 (6%)	21	33
All	All	473/486 (97%)	449 (95%)	24 (5%)	24	37

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1554	ARG
1	A	1558	HIS
1	A	1559	GLU
1	A	1569	LEU
1	A	1594	THR
1	A	1609	THR
1	A	1614	TYR
1	A	1674	ARG
1	A	1685	LEU
1	A	1779	THR
1	A	1780	LEU
1	B	1548	PHE
1	B	1549	GLU
1	B	1551	PHE
1	B	1554	ARG
1	B	1556	GLN
1	B	1558	HIS
1	B	1567	LYS
1	B	1602	LEU
1	B	1603	ILE
1	B	1614	TYR
1	B	1730	THR

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Mol	Chain	Res	Type
1	B	1743	VAL
1	B	1816	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1555	HIS
1	A	1814	GLN
1	B	1596	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
4	POP	B	1817	-	6,8,8	0.71	0	13,13,13	1.34	1 (7%)
2	PEV	B	1	-	48,48,48	1.35	8 (16%)	51,53,53	1.19	5 (9%)
2	PEV	A	1	-	48,48,48	1.34	7 (14%)	51,53,53	1.12	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POP	B	1818	-	6,8,8	0.73	0	13,13,13	1.28	1 (7%)

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
4	POP	B	1817	-	-	0/6/6/6	-
2	PEV	B	1	-	1/1/4/4	24/52/52/52	-
2	PEV	A	1	-	1/1/4/4	30/52/52/52	-
4	POP	B	1818	-	-	0/6/6/6	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	PEV	O3-C11	3.48	1.43	1.33
2	A	1	PEV	O3-C11	3.42	1.43	1.33
2	B	1	PEV	O2-C31	3.15	1.43	1.34
2	A	1	PEV	O2-C31	3.09	1.43	1.34
2	A	1	PEV	C25-C24	-2.69	1.32	1.51
2	B	1	PEV	C25-C24	-2.64	1.32	1.51
2	B	1	PEV	P-O3P	2.24	1.68	1.59
2	A	1	PEV	P-O3P	2.22	1.68	1.59
2	B	1	PEV	C32-C31	2.19	1.57	1.50
2	B	1	PEV	P-O2P	2.16	1.65	1.55
2	A	1	PEV	P-O2P	2.16	1.65	1.55
2	A	1	PEV	C32-C31	2.12	1.56	1.50
2	B	1	PEV	C3-C2	2.07	1.57	1.50
2	A	1	PEV	C48-C47	-2.04	1.33	1.49
2	B	1	PEV	C48-C47	-2.03	1.33	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PEV	O2-C31-C32	4.01	120.15	111.50
2	B	1	PEV	O2-C31-C32	3.88	119.87	111.50
4	B	1818	POP	P2-O-P1	-3.35	121.33	132.83
4	B	1817	POP	P2-O-P1	-3.27	121.61	132.83
2	B	1	PEV	O3-C3-C2	3.17	117.67	108.43
2	A	1	PEV	O3-C3-C2	3.01	117.20	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PEV	O4P-C4-C5	2.62	118.91	109.10
2	B	1	PEV	O3-C11-C12	2.54	119.87	111.91
2	A	1	PEV	O3-C11-C12	2.33	119.21	111.91
2	B	1	PEV	O4P-C4-C5	2.19	117.29	109.10
2	B	1	PEV	O2-C31-O31	-2.06	118.72	123.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	PEV	C2
2	A	1	PEV	C2

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	PEV	C32-C31-O2-C2
2	B	1	PEV	O31-C31-O2-C2
2	B	1	PEV	C5-C4-O4P-P
2	B	1	PEV	O4P-C4-C5-N6
2	A	1	PEV	C32-C31-O2-C2
2	A	1	PEV	O2-C2-C3-O3
2	A	1	PEV	C4-O4P-P-O3P
2	A	1	PEV	C4-O4P-P-O1P
2	A	1	PEV	C5-C4-O4P-P
2	B	1	PEV	O11-C11-O3-C3
2	A	1	PEV	O31-C31-O2-C2
2	B	1	PEV	C12-C11-O3-C3
2	B	1	PEV	C14-C15-C16-C17
2	B	1	PEV	C16-C17-C18-C19
2	A	1	PEV	C21-C22-C23-C24
2	B	1	PEV	C31-C32-C33-C34
2	B	1	PEV	C19-C20-C21-C22
2	A	1	PEV	C12-C13-C14-C15
2	A	1	PEV	C37-C38-C39-C40
2	A	1	PEV	C19-C20-C21-C22
2	B	1	PEV	C12-C13-C14-C15
2	B	1	PEV	C3-C2-O2-C31
2	A	1	PEV	C40-C41-C42-C43
2	A	1	PEV	C23-C24-C25-C26
2	A	1	PEV	C31-C32-C33-C34
2	A	1	PEV	C34-C35-C36-C37
2	A	1	PEV	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
2	A	1	PEV	C35-C36-C37-C38
2	A	1	PEV	C15-C16-C17-C18
2	A	1	PEV	C14-C15-C16-C17
2	B	1	PEV	C22-C23-C24-C25
2	A	1	PEV	C38-C39-C40-C41
2	B	1	PEV	C1-C2-C3-O3
2	B	1	PEV	C40-C41-C42-C43
2	B	1	PEV	C13-C14-C15-C16
2	B	1	PEV	C15-C16-C17-C18
2	B	1	PEV	C45-C46-C47-C48
2	A	1	PEV	C33-C34-C35-C36
2	B	1	PEV	O3P-C1-C2-C3
2	A	1	PEV	C32-C33-C34-C35
2	A	1	PEV	C1-O3P-P-O4P
2	A	1	PEV	C1-C2-C3-O3
2	B	1	PEV	O3P-C1-C2-O2
2	A	1	PEV	C11-C12-C13-C14
2	A	1	PEV	C36-C37-C38-C39
2	B	1	PEV	C35-C36-C37-C38
2	A	1	PEV	C16-C17-C18-C19
2	B	1	PEV	C1-O3P-P-O4P
2	A	1	PEV	O4P-C4-C5-N6
2	B	1	PEV	C17-C18-C19-C20
2	A	1	PEV	O2-C31-C32-C33
2	A	1	PEV	C20-C21-C22-C23
2	A	1	PEV	O31-C31-C32-C33
2	B	1	PEV	O31-C31-C32-C33

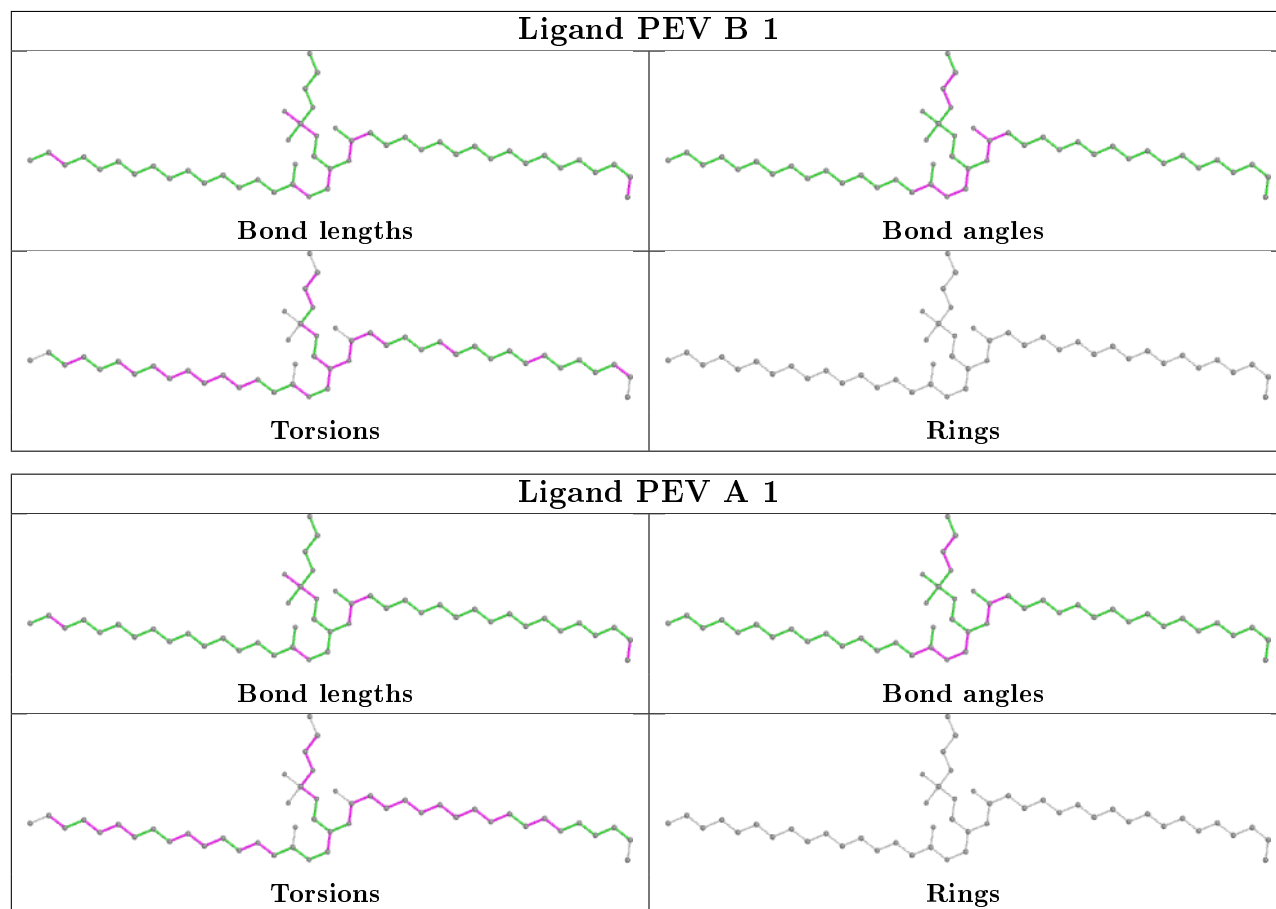
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	PEV	9	0
2	A	1	PEV	8	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	270/276 (97%)	-0.07	11 (4%) 37 33	32, 53, 112, 147	0
1	B	270/276 (97%)	-0.02	11 (4%) 37 33	27, 50, 114, 167	0
All	All	540/552 (97%)	-0.05	22 (4%) 37 33	27, 52, 115, 167	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1558	HIS	9.7
1	B	1554	ARG	6.4
1	A	1556	GLN	4.8
1	B	1555	HIS	4.1
1	A	1563	PHE	4.1
1	B	1548	PHE	3.8
1	A	1558	HIS	3.7
1	B	1547	LYS	3.5
1	B	1553	THR	3.4
1	B	1556	GLN	3.3
1	A	1553	THR	3.2
1	A	1554	ARG	3.1
1	B	1557	VAL	3.0
1	B	1775	GLU	2.9
1	A	1551	PHE	2.8
1	A	1550	GLU	2.7
1	A	1604	TYR	2.5
1	A	1560	LYS	2.5
1	B	1552	MET	2.5
1	A	1552	MET	2.1
1	B	1549	GLU	2.1
1	A	1555	HIS	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](#)

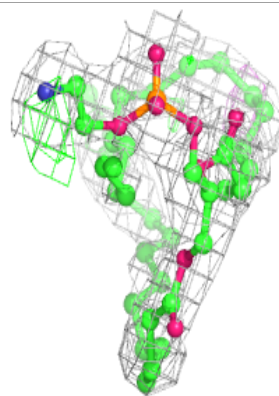
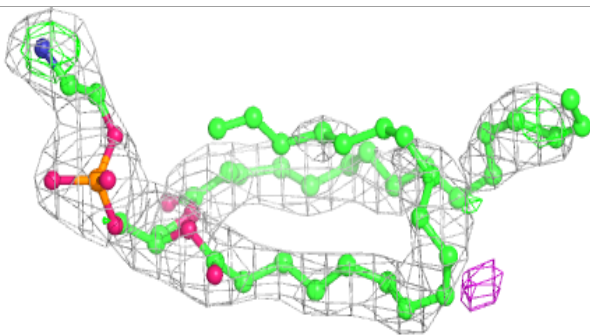
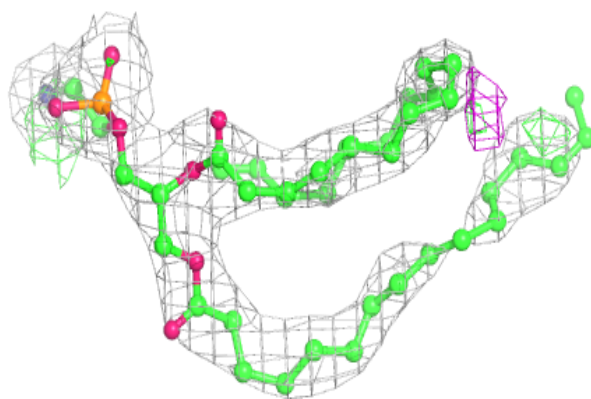
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	A	1817	1/1	0.81	0.17	68,68,68,68	1
2	PEV	A	1	49/49	0.90	0.28	25,74,112,118	3
2	PEV	B	1	49/49	0.91	0.34	24,67,192,201	3
4	POP	B	1817	9/9	0.93	0.12	82,90,108,206	0
4	POP	B	1818	9/9	0.94	0.14	60,68,83,125	0

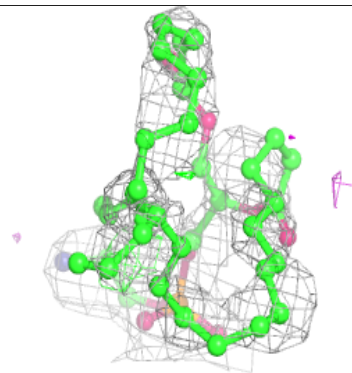
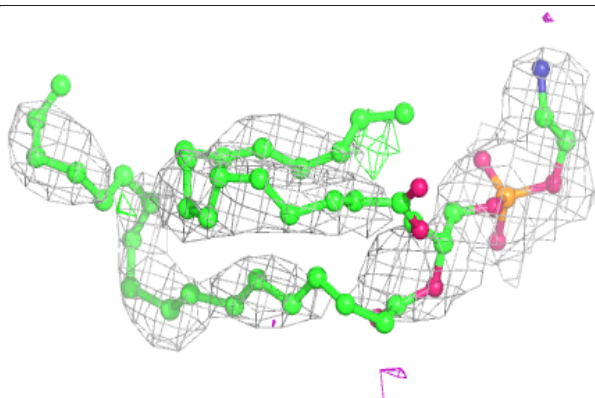
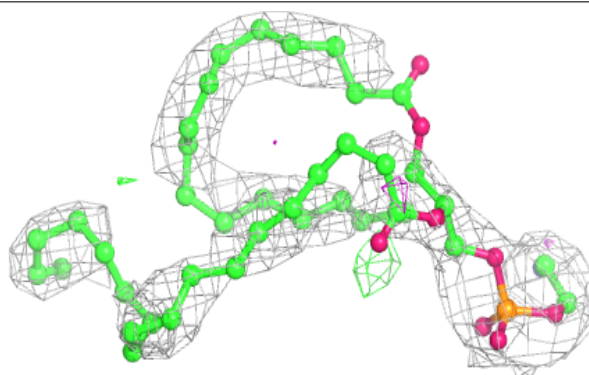
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEV A 1:

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

**Electron density around PEV B 1:**

$2mF_o-DF_c$ (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.