



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 PM UTC

PDB ID : 3PG7 / pdb_00003pg7
Title : Crystal structure of the H. sapiens NF1 SEC-PH domain (del1750 mutant)
Authors : Welti, S.; D'Angelo, I.; Scheffzek, K.
Deposited on : 2010-10-31
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

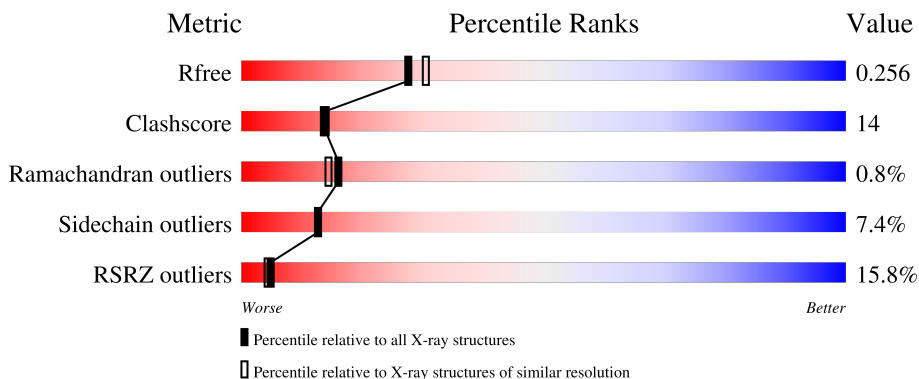
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	256	
1	B	256	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4362 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.

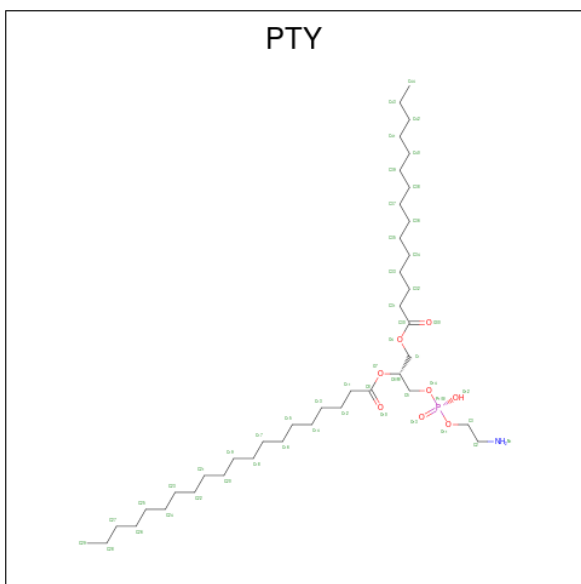
- Molecule 1 is a protein called Neurofibromin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	2002	1294	335	368	5	0	0	0
1	B	256	2009	1299	332	373	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P21359
B	?	-	LYS	deletion	UNP P21359

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



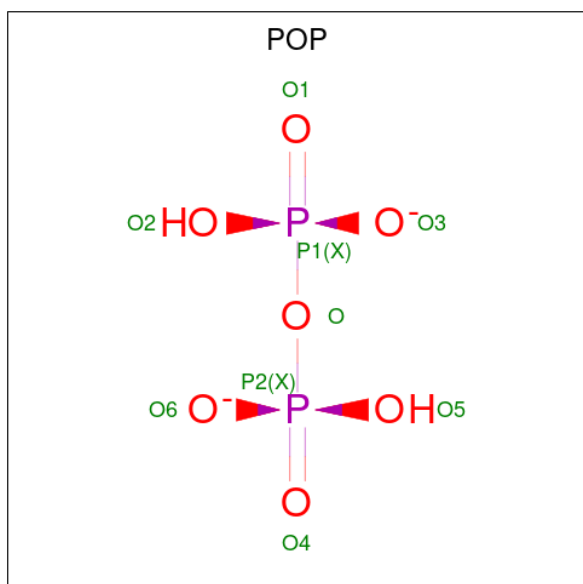
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	46	36	1	8	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	46	36	1	8	1	0	0

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $H_2O_7P_2$).



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

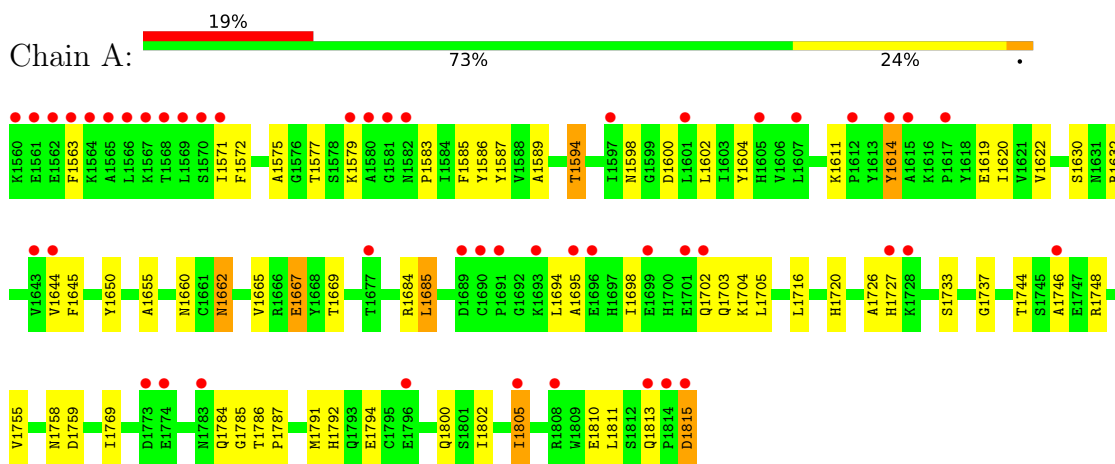
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	98	98	98	0	0
4	B	143	143	143	0	0

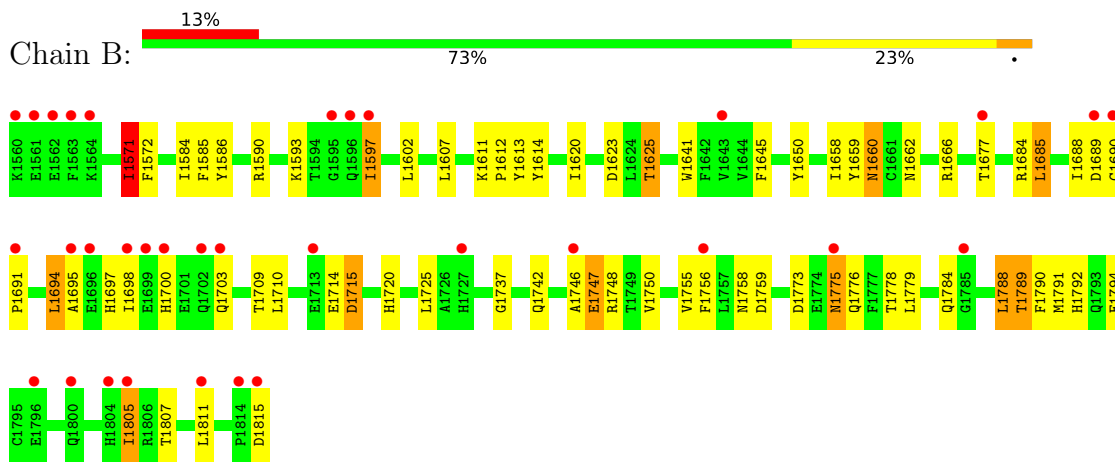
3 Residue-property plots [i](#)

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: 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	113.44Å 113.44Å 124.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 2.19 36.00 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.4 (36.00-2.19) 99.3 (36.00-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.208 , 0.249 0.212 , 0.256	Depositor DCC
R_{free} test set	2136 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtrriage
Anisotropy	0.157	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4362	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: POP, PTY

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	0.32	0/2052	0.73	0/2796
1	B	0.34	0/2059	0.75	1/2809 (0.0%)
All	All	0.33	0/4111	0.74	1/5605 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1571	ILE	CB-CA-C	-5.13	105.36	112.24

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	2002	0	1922	57	0
1	B	2009	0	1936	61	0
2	A	46	0	65	6	0
2	B	46	0	65	6	0
3	B	18	0	0	0	0
4	A	98	0	0	2	0
4	B	143	0	0	7	0
All	All	4362	0	3988	117	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 14.

All (117) 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)
2:B:500:PTY:H221	2:B:500:PTY:H381	1.31	1.06
1:A:1703:GLN:HE21	1:A:1705:LEU:H	1.11	0.97
1:B:1792:HIS:HD2	1:B:1794:GLU:H	1.17	0.92
1:A:1792:HIS:HD2	1:A:1794:GLU:H	1.20	0.88
1:B:1623:ASP:OD2	1:B:1625:THR:HG23	1.74	0.86
1:B:1700:HIS:HA	1:B:1703:GLN:HE21	1.41	0.86
1:B:1650:TYR:HD2	2:B:500:PTY:HC12	1.42	0.83
1:B:1792:HIS:CD2	1:B:1794:GLU:H	1.98	0.82
1:B:1700:HIS:HA	1:B:1703:GLN:NE2	1.97	0.79
1:A:1792:HIS:CD2	1:A:1794:GLU:H	2.07	0.72
1:A:1810:GLU:O	1:A:1813:GLN:HG2	1.89	0.72
1:B:1742:GLN:HB3	1:B:1758:ASN:HD21	1.56	0.70
1:B:1746:ALA:O	1:B:1748:ARG:HG2	1.92	0.70
1:B:1703:GLN:NE2	4:B:127:HOH:O	2.24	0.69
2:A:400:PTY:H392	2:A:400:PTY:H221	1.74	0.69
1:A:1815:ASP:HA	1:B:1590:ARG:HE	1.60	0.66
1:A:1695:ALA:HA	1:A:1698:ILE:O	1.96	0.64
1:A:1698:ILE:HG22	1:A:1702:GLN:HB3	1.78	0.64
1:A:1575:ALA:HB1	1:A:1704:LYS:HG3	1.80	0.63
1:B:1695:ALA:HA	1:B:1698:ILE:O	1.99	0.62
1:A:1662:ASN:C	1:A:1662:ASN:HD22	2.07	0.62
1:A:1662:ASN:ND2	1:A:1665:VAL:H	1.97	0.62
1:A:1667:GLU:HG2	4:A:213:HOH:O	2.00	0.62
1:B:1695:ALA:C	1:B:1697:HIS:H	2.09	0.61
1:B:1611:LYS:HB3	1:B:1612:PRO:HD3	1.83	0.61
1:B:1625:THR:HG21	1:B:1709:THR:HG23	1.83	0.60
1:A:1703:GLN:NE2	1:A:1705:LEU:H	1.90	0.60
1:B:1584:ILE:HD13	1:B:1698:ILE:HD13	1.84	0.59
1:B:1694:LEU:HB3	4:B:127:HOH:O	2.02	0.59
1:A:1720:HIS:O	1:A:1792:HIS:HE1	1.87	0.58
1:A:1577:THR:O	1:A:1702:GLN:HG2	2.04	0.58
1:B:1725:LEU:HD11	1:B:1791:MET:HG3	1.86	0.57
1:A:1650:TYR:O	1:A:1684:ARG:NH2	2.38	0.57
1:A:1611:LYS:HA	1:A:1614:TYR:CE2	2.40	0.56
1:B:1694:LEU:C	4:B:127:HOH:O	2.48	0.56
1:A:1598:ASN:HD21	1:A:1600:ASP:HB2	1.71	0.56
1:B:1792:HIS:HD2	1:B:1794:GLU:N	1.97	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1619:GLU:HG2	1:A:1655:ALA:HB3	1.87	0.55
1:A:1645:PHE:HB2	1:A:1650:TYR:CZ	2.41	0.55
1:B:1700:HIS:O	1:B:1703:GLN:HB2	2.06	0.55
1:B:1720:HIS:O	1:B:1792:HIS:HE1	1.90	0.54
1:A:1815:ASP:CG	1:B:1590:ARG:HD2	2.33	0.54
1:B:1623:ASP:OD2	1:B:1625:THR:CG2	2.51	0.53
1:A:1792:HIS:HD2	1:A:1794:GLU:N	1.99	0.53
1:B:1695:ALA:N	4:B:127:HOH:O	2.41	0.53
1:B:1775:ASN:HD22	1:B:1775:ASN:C	2.16	0.52
1:A:1662:ASN:HD21	1:A:1665:VAL:HG23	1.75	0.52
1:B:1650:TYR:O	1:B:1684:ARG:NH2	2.42	0.52
1:B:1658:ILE:HD11	1:B:1685:LEU:HD13	1.92	0.51
1:B:1695:ALA:C	1:B:1697:HIS:N	2.66	0.51
1:B:1784:GLN:NE2	4:B:237:HOH:O	2.43	0.51
1:B:1645:PHE:HB2	1:B:1650:TYR:CZ	2.45	0.51
1:B:1703:GLN:CD	4:B:127:HOH:O	2.50	0.51
1:A:1598:ASN:ND2	1:A:1600:ASP:HB2	2.25	0.51
1:B:1775:ASN:HA	1:B:1792:HIS:O	2.11	0.51
1:B:1662:ASN:HB2	1:B:1759:ASP:OD1	2.11	0.50
1:B:1641:TRP:HB3	2:B:500:PTY:H251	1.92	0.50
1:A:1587:TYR:CE2	1:A:1589:ALA:HA	2.47	0.50
1:B:1593:LYS:H	1:B:1597:ILE:HD12	1.76	0.50
1:B:1607:LEU:C	1:B:1607:LEU:HD23	2.37	0.49
1:A:1620:ILE:HG13	2:A:400:PTY:H312	1.94	0.49
1:A:1645:PHE:HB2	1:A:1650:TYR:CE1	2.48	0.49
1:A:1703:GLN:HE21	1:A:1705:LEU:N	1.95	0.49
1:A:1746:ALA:O	1:A:1748:ARG:HG2	2.13	0.48
1:A:1622:VAL:O	1:A:1622:VAL:HG23	2.12	0.48
1:B:1773:ASP:O	1:B:1775:ASN:N	2.42	0.48
1:A:1698:ILE:CG2	1:A:1702:GLN:HB3	2.41	0.48
1:A:1650:TYR:HD2	2:A:400:PTY:HC52	1.79	0.48
1:A:1650:TYR:CD2	2:A:400:PTY:HC52	2.49	0.48
1:B:1807:THR:O	1:B:1811:LEU:HG	2.14	0.48
1:A:1572:PHE:HA	1:A:1586:TYR:O	2.14	0.48
1:A:1733:SER:HB2	1:A:1744:THR:OG1	2.13	0.48
1:A:1726:ALA:O	1:A:1727:HIS:C	2.56	0.47
1:B:1666:ARG:HG3	1:B:1750:VAL:HG22	1.96	0.47
1:B:1659:TYR:HE1	1:B:1691:PRO:HA	1.79	0.47
1:A:1662:ASN:HB2	1:A:1759:ASP:OD1	2.14	0.47
2:B:500:PTY:H412	2:B:500:PTY:H201	1.96	0.47
1:B:1690:CYS:HA	4:B:99:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1815:ASP:OD1	1:B:1590:ARG:HD2	2.15	0.46
1:B:1746:ALA:O	1:B:1747:GLU:C	2.59	0.46
1:A:1737:GLY:O	1:A:1805:ILE:HG12	2.16	0.46
1:A:1685:LEU:HD23	1:A:1685:LEU:N	2.29	0.45
1:A:1660:ASN:ND2	1:A:1758:ASN:HD22	2.15	0.45
1:A:1815:ASP:HB3	1:B:1590:ARG:HG3	1.99	0.45
1:A:1694:LEU:HD23	1:A:1703:GLN:HG3	1.98	0.45
1:B:1720:HIS:O	1:B:1792:HIS:CE1	2.69	0.45
1:B:1773:ASP:C	1:B:1775:ASN:H	2.22	0.45
1:B:1778:THR:HG22	1:B:1789:THR:HB	1.99	0.45
1:B:1620:ILE:HD13	2:B:500:PTY:H332	1.99	0.45
1:B:1788:LEU:HB3	1:B:1790:PHE:CE1	2.52	0.45
1:A:1720:HIS:O	1:A:1792:HIS:CE1	2.68	0.45
1:A:1769:ILE:HD13	1:A:1802:ILE:HG22	1.99	0.44
1:A:1594:THR:HG21	1:A:1632:ARG:HG2	1.99	0.44
1:A:1585:PHE:HB2	1:A:1620:ILE:HD13	1.99	0.44
1:A:1620:ILE:HG13	2:A:400:PTY:C32	2.49	0.43
1:B:1585:PHE:HZ	1:B:1613:TYR:CD1	2.37	0.42
1:A:1815:ASP:HA	1:B:1590:ARG:NE	2.30	0.42
1:B:1572:PHE:HA	1:B:1586:TYR:O	2.19	0.42
1:A:1784:GLN:O	1:A:1786:THR:N	2.51	0.42
1:B:1571:ILE:H	1:B:1571:ILE:HD12	1.85	0.42
1:B:1688:ILE:CG2	1:B:1690:CYS:O	2.68	0.42
1:A:1662:ASN:ND2	1:A:1665:VAL:HG23	2.34	0.42
1:B:1660:ASN:HD22	1:B:1660:ASN:HA	1.64	0.42
2:B:500:PTY:H212	2:B:500:PTY:H182	1.86	0.41
1:B:1689:ASP:HB3	1:B:1756:PHE:HB2	2.02	0.41
1:B:1725:LEU:HD11	1:B:1791:MET:CG	2.48	0.41
1:A:1563:PHE:CE1	1:A:1604:TYR:HD2	2.39	0.41
1:B:1776:GLN:HE21	1:B:1791:MET:HG2	1.85	0.41
1:A:1602:LEU:HD12	1:A:1602:LEU:O	2.21	0.41
1:A:1786:THR:HA	1:A:1787:PRO:HD2	1.84	0.41
1:B:1737:GLY:O	1:B:1805:ILE:HG12	2.20	0.41
1:A:1620:ILE:HG13	2:A:400:PTY:H321	2.02	0.41
1:A:1583:PRO:HG2	4:A:74:HOH:O	2.20	0.40
1:B:1714:GLU:O	1:B:1715:ASP:C	2.64	0.40
1:A:1791:MET:HE3	1:A:1791:MET:HB2	1.97	0.40
1:A:1594:THR:HG22	1:A:1630:SER:O	2.22	0.40
1:B:1584:ILE:HD13	1:B:1698:ILE:CD1	2.51	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	254/256 (99%)	242 (95%)	11 (4%)	1 (0%)	30	31
1	B	254/256 (99%)	239 (94%)	12 (5%)	3 (1%)	10	7
All	All	508/512 (99%)	481 (95%)	23 (4%)	4 (1%)	16	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1785	GLY
1	B	1747	GLU
1	B	1597	ILE
1	B	1715	ASP

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	207/226 (92%)	192 (93%)	15 (7%)	13	13
1	B	211/226 (93%)	195 (92%)	16 (8%)	12	12
All	All	418/452 (92%)	387 (93%)	31 (7%)	13	13

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

Mol	Chain	Res	Type
1	A	1571	ILE
1	A	1579	LYS

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Mol	Chain	Res	Type
1	A	1594	THR
1	A	1614	TYR
1	A	1644	VAL
1	A	1662	ASN
1	A	1667	GLU
1	A	1669	THR
1	A	1685	LEU
1	A	1716	LEU
1	A	1755	VAL
1	A	1800	GLN
1	A	1805	ILE
1	A	1811	LEU
1	A	1815	ASP
1	B	1571	ILE
1	B	1602	LEU
1	B	1614	TYR
1	B	1625	THR
1	B	1660	ASN
1	B	1677	THR
1	B	1685	LEU
1	B	1694	LEU
1	B	1710	LEU
1	B	1755	VAL
1	B	1775	ASN
1	B	1779	LEU
1	B	1788	LEU
1	B	1789	THR
1	B	1805	ILE
1	B	1815	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1574	GLN
1	A	1598	ASN
1	A	1660	ASN
1	A	1662	ASN
1	A	1672	HIS
1	A	1702	GLN
1	A	1703	GLN
1	A	1783	ASN
1	A	1784	GLN

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Mol	Chain	Res	Type
1	A	1792	HIS
1	A	1800	GLN
1	B	1582	ASN
1	B	1660	ASN
1	B	1672	HIS
1	B	1703	GLN
1	B	1753	GLN
1	B	1758	ASN
1	B	1775	ASN
1	B	1776	GLN
1	B	1792	HIS

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POP	B	602	-	6,8,8	0.81	0	12,13,13	1.03	0
2	PTY	A	400	-	45,45,49	1.27	3 (6%)	48,50,54	1.28	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PTY	B	500	-	45,45,49	1.23	3 (6%)	48,50,54	1.29	5 (10%)
3	POP	B	601	-	6,8,8	0.75	0	12,13,13	0.97	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	POP	B	602	-	-	0/6/6/6	-
2	PTY	A	400	-	-	16/49/49/53	-
2	PTY	B	500	-	-	20/49/49/53	-
3	POP	B	601	-	-	1/6/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	PTY	O4-C30	3.87	1.44	1.33
2	B	500	PTY	O4-C30	3.74	1.44	1.33
2	A	400	PTY	O7-C8	3.10	1.43	1.34
2	B	500	PTY	O7-C8	3.01	1.42	1.34
2	B	500	PTY	P1-O12	2.15	1.65	1.55
2	A	400	PTY	P1-O12	2.13	1.65	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PTY	O7-C8-C11	4.11	120.38	111.48
2	B	500	PTY	O7-C8-C11	4.07	120.28	111.48
2	B	500	PTY	O4-C1-C6	3.58	118.72	108.40
2	A	400	PTY	O4-C1-C6	3.57	118.68	108.40
2	B	500	PTY	O4-C30-C31	3.18	121.54	111.83
2	A	400	PTY	O4-C30-C31	2.81	120.41	111.83
2	A	400	PTY	O11-C3-C2	2.73	119.16	109.17
2	B	500	PTY	O11-C3-C2	2.50	118.32	109.17
2	B	500	PTY	O7-C6-C5	2.21	116.26	108.34

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	PTY	O14-C5-C6-O7
3	B	601	POP	P2-O-P1-O2
2	B	500	PTY	C18-C19-C20-C21
2	B	500	PTY	C32-C33-C34-C35
2	A	400	PTY	C33-C34-C35-C36
2	B	500	PTY	C17-C18-C19-C20
2	A	400	PTY	O30-C30-O4-C1
2	A	400	PTY	C13-C14-C15-C16
2	A	400	PTY	C11-C8-O7-C6
2	B	500	PTY	C11-C8-O7-C6
2	B	500	PTY	O4-C1-C6-O7
2	A	400	PTY	C32-C33-C34-C35
2	B	500	PTY	C14-C15-C16-C17
2	A	400	PTY	C39-C40-C41-C42
2	A	400	PTY	C17-C18-C19-C20
2	A	400	PTY	O10-C8-O7-C6
2	A	400	PTY	C18-C19-C20-C21
2	B	500	PTY	C36-C37-C38-C39
2	B	500	PTY	C40-C41-C42-C43
2	B	500	PTY	C16-C17-C18-C19
2	A	400	PTY	C31-C30-O4-C1
2	B	500	PTY	C33-C34-C35-C36
2	B	500	PTY	O14-C5-C6-C1
2	B	500	PTY	C23-C24-C25-C26
2	B	500	PTY	C34-C35-C36-C37
2	B	500	PTY	C30-C31-C32-C33
2	A	400	PTY	C3-O11-P1-O13
2	A	400	PTY	C5-O14-P1-O13
2	A	400	PTY	C35-C36-C37-C38
2	A	400	PTY	C19-C20-C21-C22
2	B	500	PTY	C1-C6-O7-C8
2	A	400	PTY	C12-C13-C14-C15
2	B	500	PTY	C12-C11-C8-O7
2	B	500	PTY	C12-C11-C8-O10
2	B	500	PTY	O30-C30-C31-C32
2	B	500	PTY	O4-C30-C31-C32
2	A	400	PTY	O4-C30-C31-C32

There are no ring outliers.

2 monomers are involved in 12 short contacts:

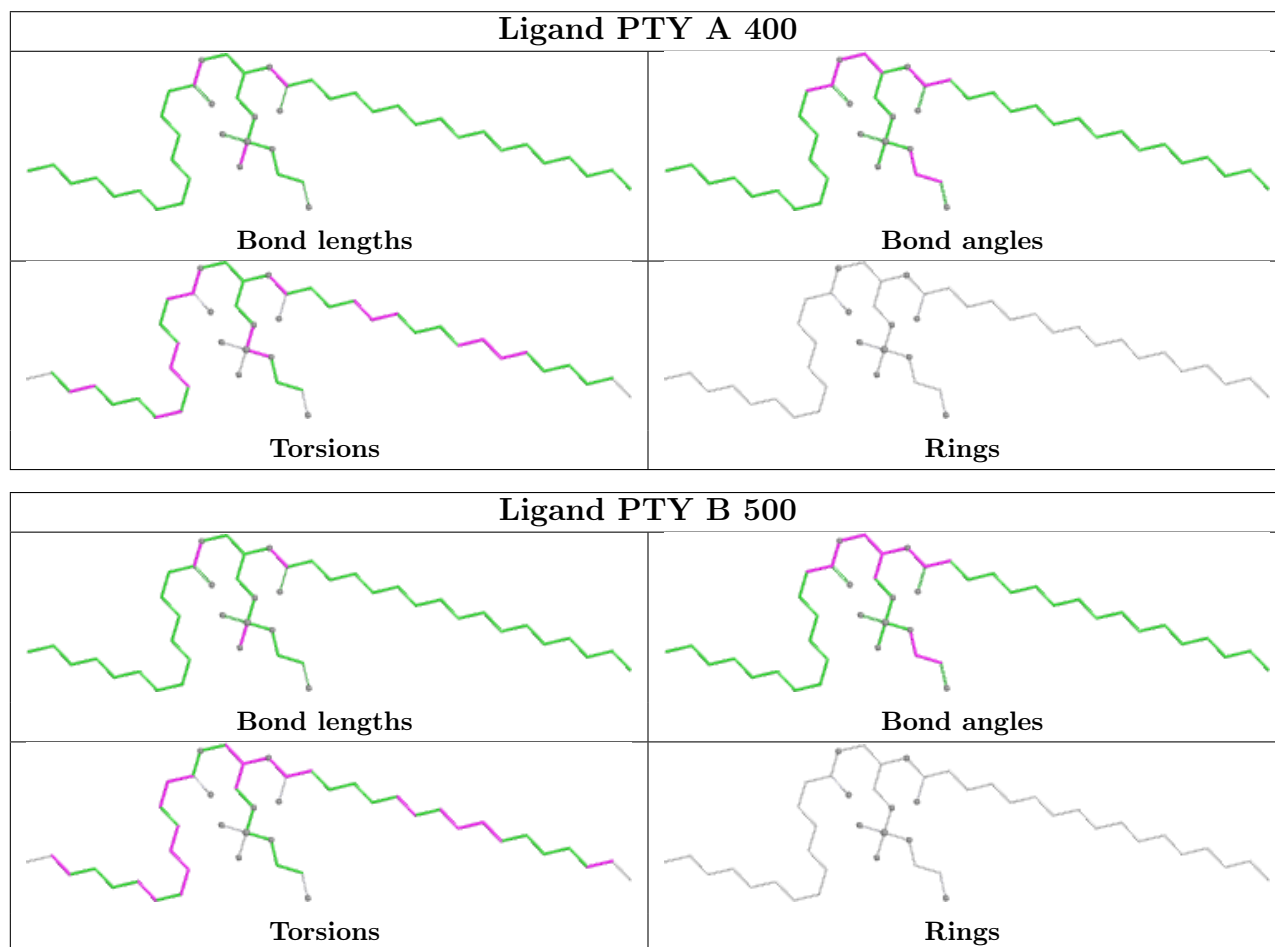
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	PTY	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	PTY	6	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

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	256/256 (100%)	0.90	48 (18%) 3 3	29, 53, 92, 118	0
1	B	256/256 (100%)	0.55	33 (12%) 7 6	25, 46, 78, 110	0
All	All	512/512 (100%)	0.73	81 (15%) 5 4	25, 49, 88, 118	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1696	GLU	6.2
1	A	1814	PRO	5.1
1	B	1689	ASP	5.0
1	B	1560	LYS	5.0
1	B	1796	GLU	4.8
1	B	1814	PRO	4.8
1	B	1815	ASP	4.7
1	B	1561	GLU	4.5
1	A	1563	PHE	4.5
1	A	1727	HIS	4.4
1	B	1563	PHE	4.3
1	A	1615	ALA	4.2
1	A	1564	LYS	4.2
1	A	1581	GLY	4.1
1	A	1560	LYS	4.1
1	A	1691	PRO	4.1
1	A	1815	ASP	4.0
1	B	1690	CYS	4.0
1	A	1702	GLN	3.9
1	A	1690	CYS	3.8
1	B	1804	HIS	3.8
1	A	1597	ILE	3.7
1	A	1568	THR	3.7
1	A	1644	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1562	GLU	3.7
1	A	1695	ALA	3.5
1	A	1813	GLN	3.5
1	A	1569	LEU	3.5
1	A	1699	GLU	3.4
1	A	1805	ILE	3.2
1	B	1698	ILE	3.2
1	A	1701	GLU	3.2
1	A	1607	LEU	3.1
1	A	1746	ALA	3.1
1	B	1562	GLU	3.1
1	B	1700	HIS	3.1
1	B	1691	PRO	3.1
1	B	1643	VAL	3.1
1	B	1746	ALA	3.1
1	A	1566	LEU	3.0
1	A	1567	LYS	3.0
1	B	1699	GLU	3.0
1	B	1756	PHE	2.9
1	A	1643	VAL	2.8
1	A	1580	ALA	2.8
1	A	1571	ILE	2.8
1	A	1696	GLU	2.7
1	A	1561	GLU	2.7
1	A	1808	ARG	2.7
1	A	1693	LYS	2.6
1	B	1785	GLY	2.6
1	A	1570	SER	2.6
1	A	1773	ASP	2.6
1	B	1811	LEU	2.6
1	A	1565	ALA	2.5
1	B	1775	ASN	2.5
1	B	1596	GLN	2.5
1	A	1774	GLU	2.4
1	A	1677	THR	2.4
1	B	1703	GLN	2.4
1	A	1728	LYS	2.4
1	A	1605	HIS	2.4
1	B	1597	ILE	2.3
1	A	1617	PRO	2.3
1	B	1677	THR	2.3
1	B	1595	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1805	ILE	2.3
1	B	1695	ALA	2.2
1	A	1579	LYS	2.2
1	A	1783	ASN	2.2
1	A	1612	PRO	2.2
1	A	1689	ASP	2.2
1	A	1796	GLU	2.1
1	B	1713	GLU	2.1
1	A	1614	TYR	2.1
1	B	1727	HIS	2.1
1	B	1564	LYS	2.1
1	B	1702	GLN	2.1
1	A	1601	LEU	2.1
1	A	1582	ASN	2.0
1	B	1800	GLN	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](#)

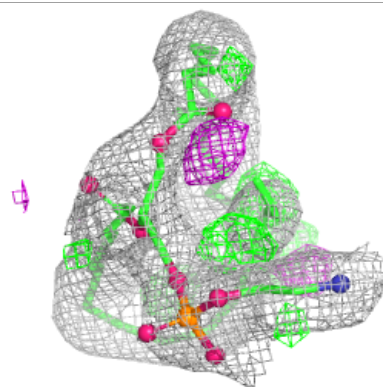
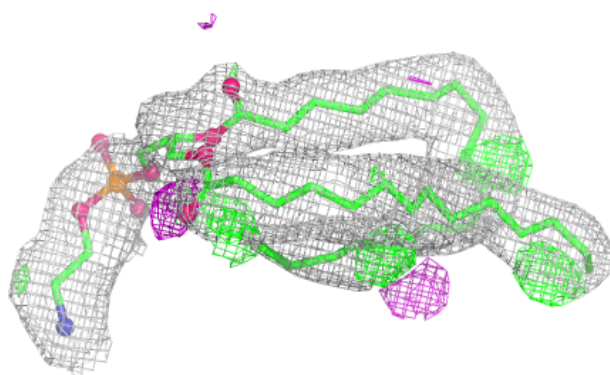
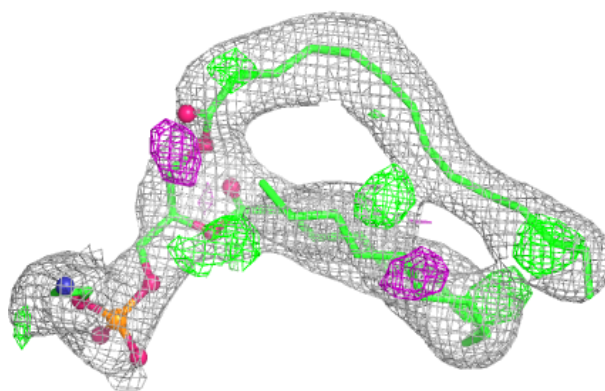
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	POP	B	601	9/9	0.72	0.20	79,94,124,127	0
3	POP	B	602	9/9	0.80	0.21	43,75,93,133	0
2	PTY	B	500	46/50	0.86	0.19	37,64,97,111	0
2	PTY	A	400	46/50	0.87	0.16	38,60,83,132	0

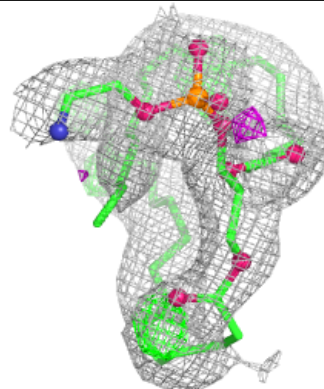
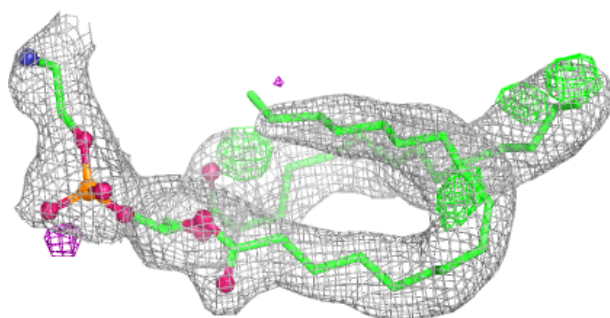
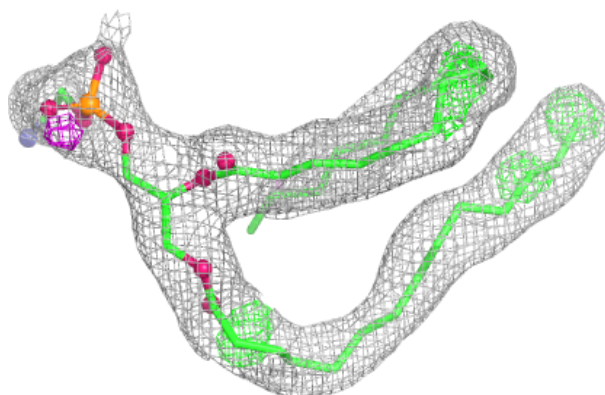
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY B 500:

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

**Electron density around PTY A 400:**

$2mF_o-DF_c$ (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.