



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:20 AM UTC

PDB ID : 2E2X / pdb\_00002e2x  
Title : Sec14 Homology Module of Neurofibromin in complex with phosphatyletha  
nolamine  
Authors : D'Angelo, I.; Welti, S.; Scheffzek, K.  
Deposited on : 2006-11-18  
Resolution : 2.50 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>.

---

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)  
Xtrriage (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

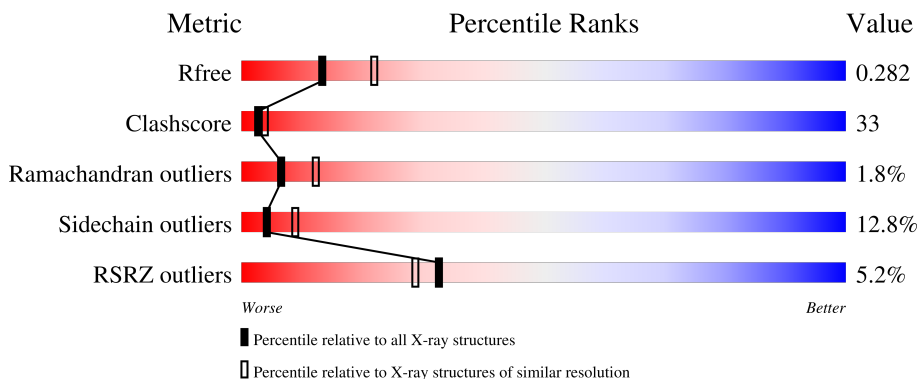
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	277	
1	B	277	

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	400	X	-	-	-
2	PEV	B	500	X	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4218 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.

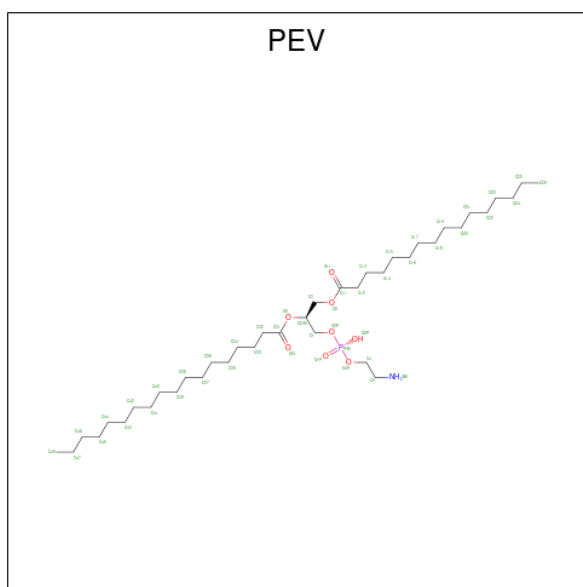
- Molecule 1 is a protein called Neurofibromin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	2013	1302	336	370	5	0	0	0
1	B	250	2015	1303	336	371	5	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

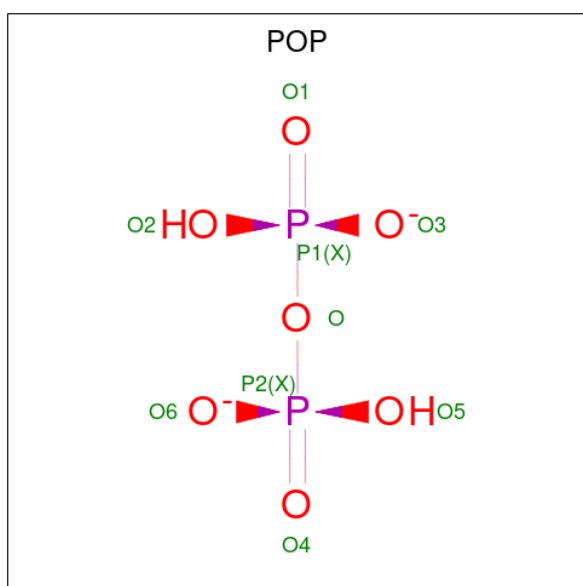
Chain	Residue	Modelled	Actual	Comment	Reference
A	1540	GLY	-	expression tag	UNP P21359
A	1541	ALA	-	expression tag	UNP P21359
A	1542	MET	-	expression tag	UNP P21359
A	1543	THR	-	expression tag	UNP P21359
A	1544	GLY	-	expression tag	UNP P21359
B	1540	GLY	-	expression tag	UNP P21359
B	1541	ALA	-	expression tag	UNP P21359
B	1542	MET	-	expression tag	UNP P21359
B	1543	THR	-	expression tag	UNP P21359
B	1544	GLY	-	expression tag	UNP P21359

- Molecule 2 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(PALMITOYL)OXY]METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



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

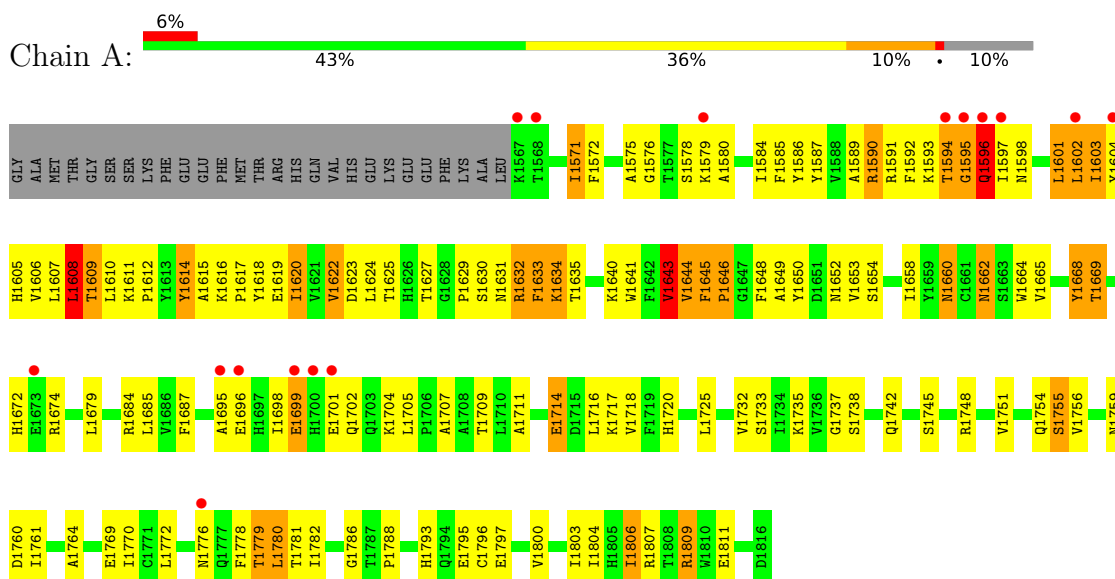
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	30	Total 30	O 30	0	0
4	B	44	Total 44	O 44	0	0

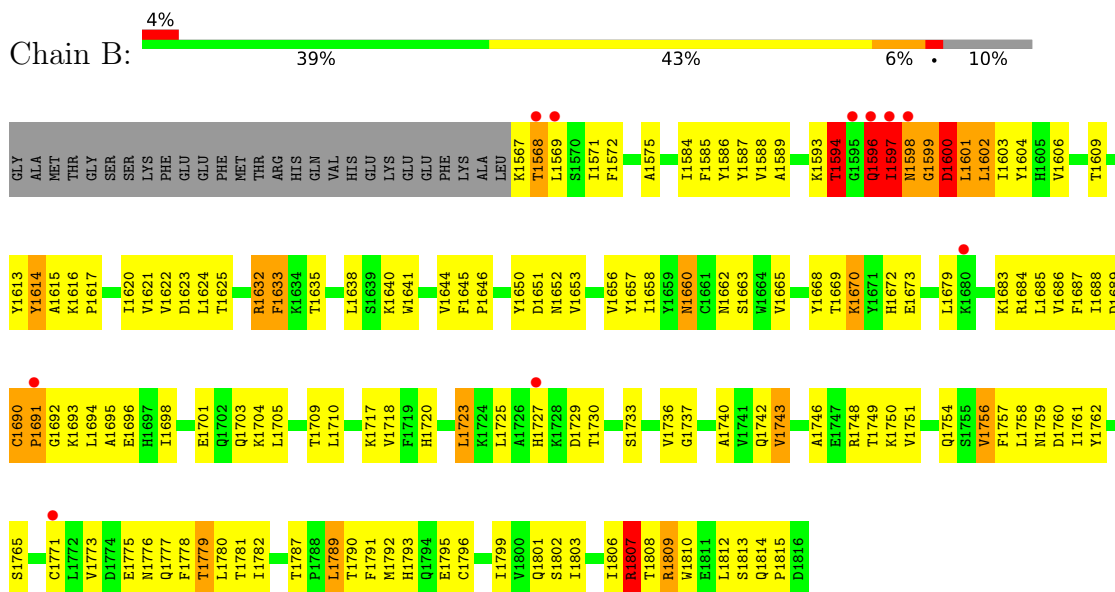
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	110.10Å 110.10Å 121.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 99.0 (15.00-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.50Å)	Xtrriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, $R_{free}$	0.254 , 0.283 0.265 , 0.282	Depositor DCC
$R_{free}$ test set	2411 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: POP, PEV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.59	0/2063	1.09	21/2801 (0.7%)
1	B	0.77	3/2065 (0.1%)	1.29	35/2804 (1.2%)
All	All	0.69	3/4128 (0.1%)	1.19	56/5605 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1597	ILE	CA-CB	6.77	1.63	1.54
1	B	1596	GLN	C-N	-6.60	1.26	1.33
1	B	1596	GLN	CG-CD	5.40	1.65	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1599	GLY	CA-C-N	-13.81	99.76	122.54
1	B	1599	GLY	C-N-CA	-13.81	99.76	122.54
1	B	1601	LEU	N-CA-C	-11.06	98.75	111.03
1	B	1690	CYS	CA-C-N	9.23	131.38	119.84
1	B	1690	CYS	C-N-CA	9.23	131.38	119.84
1	A	1646	PRO	N-CA-C	-8.59	97.57	111.15
1	B	1597	ILE	CA-C-N	-8.39	108.20	120.28
1	B	1597	ILE	C-N-CA	-8.39	108.20	120.28
1	B	1815	PRO	N-CA-C	7.33	122.01	110.50
1	A	1571	ILE	N-CA-C	-6.83	104.19	110.82
1	B	1796	CYS	N-CA-C	6.82	118.71	111.28
1	A	1615	ALA	N-CA-C	-6.71	104.11	112.90
1	B	1594	THR	N-CA-C	6.67	119.64	110.24
1	B	1751	VAL	N-CA-C	-6.53	98.05	107.78
1	A	1733	SER	N-CA-C	-6.48	99.15	109.59
1	B	1600	ASP	CA-C-O	6.41	126.85	119.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1668	TYR	N-CA-C	-6.37	104.42	111.36
1	A	1603	ILE	N-CA-C	-6.34	103.16	112.04
1	A	1595	GLY	N-CA-C	-6.24	98.40	113.18
1	A	1633	PHE	N-CA-C	-5.99	98.76	108.52
1	A	1718	VAL	N-CA-C	5.96	116.52	108.17
1	B	1604	TYR	N-CA-C	-5.92	104.77	112.23
1	A	1645	PHE	CA-C-N	5.92	125.93	119.90
1	A	1645	PHE	C-N-CA	5.92	125.93	119.90
1	B	1633	PHE	N-CA-C	-5.86	99.18	108.73
1	B	1597	ILE	CA-C-O	-5.80	114.20	120.47
1	B	1718	VAL	N-CA-C	5.79	116.44	107.99
1	B	1717	LYS	N-CA-C	-5.73	99.18	108.41
1	B	1740	ALA	N-CA-C	5.63	116.82	108.60
1	A	1751	VAL	N-CA-C	-5.58	99.47	107.78
1	A	1632	ARG	N-CA-C	5.53	117.46	110.33
1	B	1598	ASN	CA-C-N	-5.53	111.12	120.79
1	B	1598	ASN	C-N-CA	-5.53	111.12	120.79
1	B	1809	ARG	N-CA-C	-5.49	105.29	111.28
1	A	1770	ILE	N-CA-C	-5.44	100.50	108.11
1	B	1621	VAL	N-CA-C	-5.44	99.92	107.80
1	B	1733	SER	N-CA-C	-5.41	100.08	108.90
1	B	1746	ALA	N-CA-C	-5.41	106.52	113.23
1	B	1807	ARG	N-CA-C	-5.40	105.47	111.36
1	B	1599	GLY	N-CA-C	-5.38	107.99	114.66
1	B	1737	GLY	N-CA-C	-5.37	102.23	111.57
1	B	1781	THR	N-CA-C	-5.35	100.46	109.07
1	B	1670	LYS	N-CA-C	-5.31	105.16	111.69
1	A	1717	LYS	N-CA-C	-5.25	99.95	108.41
1	A	1608	LEU	N-CA-C	5.25	118.85	112.23
1	A	1714	GLU	N-CA-C	5.25	118.30	109.95
1	B	1615	ALA	N-CA-C	-5.22	106.96	113.38
1	B	1727	HIS	N-CA-C	-5.20	104.87	111.11
1	A	1705	LEU	N-CA-C	-5.17	102.65	109.84
1	B	1748	ARG	N-CA-C	5.09	117.25	110.53
1	A	1707	ALA	N-CA-C	-5.07	105.64	111.07
1	B	1632	ARG	N-CA-C	5.03	117.02	110.43
1	B	1705	LEU	N-CA-C	-5.03	103.14	110.08
1	A	1580	ALA	N-CA-C	-5.01	107.16	113.28
1	A	1609	THR	N-CA-C	-5.01	107.17	113.28
1	B	1596	GLN	CA-C-O	5.01	127.67	120.51

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	2013	0	1994	119	0
1	B	2015	0	1999	140	0
2	A	49	0	77	17	0
2	B	49	0	77	49	0
3	B	18	0	0	2	0
4	A	30	0	0	4	0
4	B	44	0	0	3	0
All	All	4218	0	4147	274	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 33.

All (274) 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:1620:ILE:CD1	2:B:500:PEV:H131	1.47	1.43
1:B:1620:ILE:CD1	2:B:500:PEV:C13	2.13	1.26
1:B:1620:ILE:CD1	2:B:500:PEV:C12	2.34	1.06
1:B:1679:LEU:CD2	2:B:500:PEV:H322	1.84	1.05
1:A:1634:LYS:HE3	1:A:1634:LYS:H	1.23	1.04
1:B:1620:ILE:CD1	2:B:500:PEV:H122	1.91	1.01
1:B:1620:ILE:HD11	2:B:500:PEV:C12	1.90	0.98
1:B:1679:LEU:HD21	2:B:500:PEV:H322	1.44	0.97
1:B:1620:ILE:HD13	2:B:500:PEV:C13	1.85	0.97
1:B:1593:LYS:O	1:B:1598:ASN:ND2	1.97	0.95
1:B:1623:ASP:OD2	1:B:1625:THR:HG23	1.66	0.95
1:A:1611:LYS:HB3	1:A:1612:PRO:CD	2.01	0.90
1:B:1620:ILE:HD13	2:B:500:PEV:H131	0.92	0.89
1:B:1625:THR:HG21	1:B:1709:THR:HG23	1.52	0.89
1:B:1690:CYS:HB3	1:B:1693:LYS:HG3	1.55	0.88
1:B:1600:ASP:HA	1:B:1603:ILE:HG22	1.57	0.87
1:B:1620:ILE:HD12	2:B:500:PEV:H122	1.57	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:LEU:O	1:A:1606:VAL:HG23	1.74	0.85
1:A:1662:ASN:HD21	1:A:1665:VAL:HG23	1.41	0.85
1:B:1690:CYS:O	1:B:1693:LYS:N	2.10	0.84
1:A:1779:THR:HG22	4:A:1836:HOH:O	1.76	0.83
1:A:1605:HIS:O	1:A:1609:THR:HG23	1.78	0.82
1:B:1620:ILE:HD12	2:B:500:PEV:C13	2.06	0.81
1:A:1634:LYS:HE3	1:A:1634:LYS:N	1.97	0.80
1:B:1690:CYS:O	1:B:1692:GLY:N	2.15	0.80
1:A:1594:THR:HG21	1:A:1632:ARG:HG2	1.62	0.79
1:B:1679:LEU:HD21	2:B:500:PEV:C32	2.10	0.79
1:B:1742:GLN:HG2	1:B:1761:ILE:HG12	1.63	0.79
1:B:1650:TYR:CD2	2:B:500:PEV:H12	2.20	0.77
1:B:1679:LEU:CD2	2:B:500:PEV:C32	2.63	0.77
1:B:1620:ILE:HD11	2:B:500:PEV:H122	1.56	0.77
1:B:1694:LEU:HD21	1:B:1698:ILE:HD12	1.66	0.76
1:A:1607:LEU:CD1	1:A:1645:PHE:CE1	2.69	0.75
1:B:1587:TYR:CE2	2:B:500:PEV:H192	2.22	0.75
1:A:1660:ASN:ND2	1:A:1759:ASN:HD22	1.85	0.75
1:A:1634:LYS:H	1:A:1634:LYS:CE	1.99	0.74
1:A:1640:LYS:O	1:A:1644:VAL:HB	1.86	0.74
1:B:1650:TYR:HB3	2:B:500:PEV:H11	1.70	0.74
1:A:1793:HIS:CD2	1:A:1795:GLU:H	2.05	0.74
1:A:1624:LEU:HD13	1:A:1665:VAL:HG11	1.70	0.74
1:B:1653:VAL:O	1:B:1684:ARG:HD2	1.89	0.73
2:B:500:PEV:O2P	4:B:1829:HOH:O	2.06	0.73
1:A:1607:LEU:HD13	1:A:1645:PHE:CE1	2.25	0.72
1:B:1720:HIS:O	1:B:1793:HIS:HE1	1.72	0.72
1:A:1587:TYR:CE2	2:A:400:PEV:H192	2.24	0.71
1:A:1594:THR:HB	1:A:1634:LYS:HE2	1.72	0.71
1:B:1602:LEU:O	1:B:1602:LEU:HD22	1.91	0.71
1:B:1789:LEU:HB3	1:B:1791:PHE:CE1	2.26	0.70
1:A:1611:LYS:HB3	1:A:1612:PRO:HD3	1.74	0.69
1:A:1592:PHE:CD1	1:A:1602:LEU:HD22	2.28	0.68
1:A:1620:ILE:HD12	2:A:400:PEV:H131	1.74	0.68
1:B:1679:LEU:HD22	2:B:500:PEV:H322	1.71	0.68
1:B:1587:TYR:CD2	2:B:500:PEV:H192	2.28	0.68
1:A:1807:ARG:O	1:A:1811:GLU:HG3	1.93	0.68
1:B:1743:VAL:HG21	4:B:1834:HOH:O	1.93	0.67
1:A:1611:LYS:HB3	1:A:1612:PRO:HD2	1.77	0.67
1:A:1590:ARG:NH2	1:A:1709:THR:OG1	2.28	0.67
1:A:1669:THR:CG2	4:A:1839:HOH:O	2.42	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1679:LEU:HD21	2:B:500:PEV:C31	2.24	0.66
1:A:1687:PHE:CG	1:A:1756:VAL:HG11	2.31	0.66
1:A:1617:PRO:HA	1:A:1652:ASN:HB3	1.77	0.66
1:B:1689:ASP:HB3	1:B:1757:PHE:HD2	1.59	0.66
1:B:1620:ILE:HD12	2:B:500:PEV:C12	2.13	0.65
1:A:1587:TYR:CD2	2:A:400:PEV:H192	2.32	0.65
1:A:1614:TYR:CZ	1:A:1646:PRO:HG2	2.32	0.65
1:A:1669:THR:HG22	4:A:1839:HOH:O	1.96	0.64
1:A:1611:LYS:HE2	1:A:1614:TYR:OH	1.98	0.64
1:B:1650:TYR:HD2	2:B:500:PEV:H12	1.59	0.64
1:A:1662:ASN:HB2	1:A:1760:ASP:OD1	1.98	0.64
1:B:1599:GLY:O	1:B:1603:ILE:HG22	1.96	0.64
1:A:1650:TYR:HD2	2:A:400:PEV:H12	1.63	0.63
1:B:1633:PHE:CZ	2:B:500:PEV:H191	2.33	0.63
1:B:1754:GLN:HG3	4:B:1844:HOH:O	1.98	0.63
1:B:1771:CYS:HB3	1:B:1779:THR:OG1	1.99	0.63
1:A:1587:TYR:HE1	1:A:1602:LEU:HD11	1.63	0.62
1:B:1602:LEU:HD13	1:B:1641:TRP:HZ2	1.63	0.62
1:A:1732:VAL:HG12	1:A:1745:SER:HA	1.79	0.62
1:B:1645:PHE:HB2	1:B:1650:TYR:CZ	2.35	0.62
1:B:1793:HIS:HD2	1:B:1795:GLU:H	1.48	0.61
1:A:1623:ASP:OD1	1:A:1709:THR:OG1	2.15	0.61
1:B:1690:CYS:C	1:B:1692:GLY:H	2.08	0.60
1:B:1602:LEU:HD13	1:B:1641:TRP:CZ2	2.36	0.60
1:B:1632:ARG:NE	3:B:602:POP:O3	2.27	0.60
1:A:1650:TYR:HB3	2:A:400:PEV:H11	1.83	0.60
1:B:1603:ILE:HD11	1:B:1644:VAL:HG21	1.84	0.60
1:B:1720:HIS:O	1:B:1793:HIS:CE1	2.54	0.59
1:B:1723:LEU:HD21	1:B:1729:ASP:HB3	1.84	0.59
1:B:1633:PHE:HB2	1:B:1668:TYR:OH	2.03	0.58
1:B:1653:VAL:HG21	2:B:500:PEV:O3	2.03	0.58
1:B:1694:LEU:HD23	1:B:1694:LEU:O	2.03	0.58
1:B:1793:HIS:CD2	1:B:1795:GLU:H	2.22	0.58
2:A:400:PEV:H321	2:A:400:PEV:H461	1.85	0.58
1:B:1640:LYS:O	1:B:1644:VAL:HG22	2.03	0.58
1:A:1587:TYR:CE2	1:A:1589:ALA:HA	2.39	0.58
2:B:500:PEV:H371	2:B:500:PEV:H412	1.86	0.57
1:A:1779:THR:HG23	1:A:1788:PRO:HB2	1.86	0.57
2:A:400:PEV:H371	2:A:400:PEV:H412	1.86	0.57
1:B:1679:LEU:CD2	2:B:500:PEV:C31	2.82	0.57
1:A:1650:TYR:CD2	2:A:400:PEV:H12	2.39	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1687:PHE:CG	1:B:1756:VAL:HG11	2.39	0.57
1:A:1644:VAL:HG13	1:A:1644:VAL:O	2.04	0.57
1:B:1568:THR:HA	1:B:1571:ILE:HD12	1.87	0.57
1:B:1620:ILE:HD11	2:B:500:PEV:C13	2.16	0.57
1:B:1690:CYS:C	1:B:1692:GLY:N	2.61	0.56
2:B:500:PEV:H461	2:B:500:PEV:H321	1.85	0.56
1:A:1571:ILE:HG21	1:A:1602:LEU:HD13	1.88	0.56
1:B:1723:LEU:CD2	1:B:1729:ASP:HB3	2.35	0.56
1:B:1679:LEU:CD1	2:B:500:PEV:H322	2.35	0.56
1:A:1643:VAL:HG13	1:A:1643:VAL:O	2.05	0.56
1:B:1742:GLN:HB3	1:B:1759:ASN:HD21	1.71	0.56
2:A:400:PEV:H202	2:A:400:PEV:H411	1.89	0.55
1:B:1588:VAL:HA	1:B:1623:ASP:HB3	1.87	0.55
1:A:1618:TYR:CZ	1:A:1653:VAL:HG22	2.41	0.55
1:B:1585:PHE:HE2	1:B:1609:THR:HG22	1.71	0.55
1:A:1579:LYS:HD2	1:A:1696:GLU:O	2.07	0.55
1:A:1575:ALA:HB1	1:A:1704:LYS:HG3	1.88	0.55
1:A:1572:PHE:CZ	1:A:1585:PHE:HB3	2.42	0.55
1:B:1736:VAL:CG1	1:B:1806:ILE:HD13	2.37	0.55
2:B:500:PEV:H202	2:B:500:PEV:H411	1.89	0.54
1:B:1679:LEU:HD22	2:B:500:PEV:C32	2.36	0.54
1:B:1572:PHE:HA	1:B:1586:TYR:O	2.08	0.54
1:B:1679:LEU:HD13	2:B:500:PEV:H342	1.89	0.54
1:A:1596:GLN:O	1:A:1598:ASN:N	2.40	0.54
1:A:1698:ILE:HG22	1:A:1699:GLU:N	2.23	0.53
1:A:1662:ASN:ND2	1:A:1665:VAL:H	2.06	0.53
1:B:1594:THR:HG23	1:B:1632:ARG:O	2.08	0.53
1:B:1650:TYR:HA	2:B:500:PEV:H32	1.89	0.53
1:B:1625:THR:HG22	1:B:1660:ASN:HB2	1.91	0.53
1:B:1635:THR:OG1	1:B:1672:HIS:HE1	1.92	0.52
1:B:1736:VAL:HG13	1:B:1806:ILE:HD13	1.90	0.52
1:A:1643:VAL:O	1:A:1643:VAL:CG1	2.56	0.52
1:A:1702:GLN:HG3	1:A:1704:LYS:HE2	1.91	0.52
2:A:400:PEV:H441	2:A:400:PEV:H341	1.92	0.52
1:A:1576:GLY:HA3	4:A:1817:HOH:O	2.10	0.51
1:A:1603:ILE:O	1:A:1607:LEU:HB2	2.11	0.51
1:A:1660:ASN:ND2	1:A:1759:ASN:ND2	2.54	0.51
1:B:1597:ILE:O	1:B:1598:ASN:C	2.52	0.51
1:B:1725:LEU:HD11	1:B:1792:MET:SD	2.50	0.51
1:A:1624:LEU:CD1	1:A:1665:VAL:HG11	2.39	0.51
1:A:1607:LEU:CD1	1:A:1645:PHE:CD1	2.94	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1645:PHE:HB2	1:A:1650:TYR:CZ	2.46	0.51
1:B:1585:PHE:CE2	1:B:1609:THR:HG22	2.45	0.51
1:A:1635:THR:OG1	1:A:1672:HIS:HE1	1.94	0.50
1:A:1662:ASN:C	1:A:1662:ASN:HD22	2.17	0.50
2:B:500:PEV:H441	2:B:500:PEV:H341	1.92	0.50
1:A:1598:ASN:O	1:A:1601:LEU:HB2	2.12	0.50
1:B:1658:ILE:HD11	1:B:1685:LEU:HD13	1.92	0.50
1:A:1776:ASN:HA	1:A:1796:CYS:HB2	1.93	0.50
1:B:1585:PHE:HZ	1:B:1613:TYR:CD1	2.29	0.50
1:B:1641:TRP:HB3	2:B:500:PEV:H471	1.94	0.50
1:B:1663:SER:HA	1:B:1758:LEU:HD13	1.95	0.49
1:B:1688:ILE:HG21	1:B:1694:LEU:HB2	1.95	0.49
1:B:1750:LYS:HA	1:B:1754:GLN:O	2.13	0.49
1:B:1587:TYR:CE2	2:B:500:PEV:H212	2.48	0.49
1:A:1742:GLN:HG2	1:A:1761:ILE:HG12	1.95	0.49
1:B:1584:ILE:HD13	1:B:1698:ILE:HD13	1.94	0.49
1:A:1589:ALA:O	1:A:1631:ASN:HB3	2.13	0.49
1:B:1567:LYS:C	1:B:1569:LEU:H	2.21	0.48
1:A:1585:PHE:HB2	1:A:1620:ILE:HD13	1.94	0.48
3:B:602:POP:O1	3:B:602:POP:O6	2.30	0.48
1:A:1635:THR:OG1	1:A:1672:HIS:CE1	2.67	0.48
1:B:1799:ILE:O	1:B:1803:ILE:HG13	2.14	0.48
1:B:1650:TYR:HD2	2:B:500:PEV:C3	2.27	0.48
1:B:1650:TYR:CE1	2:B:500:PEV:N6	2.82	0.47
1:A:1737:GLY:O	1:A:1806:ILE:HG12	2.13	0.47
1:A:1778:PHE:HE1	1:A:1780:LEU:HG	1.78	0.47
1:B:1625:THR:HG22	1:B:1660:ASN:CB	2.45	0.47
1:B:1650:TYR:CD1	2:B:500:PEV:N6	2.83	0.47
1:B:1808:THR:O	1:B:1812:LEU:HG	2.14	0.47
1:B:1622:VAL:HG21	2:B:500:PEV:H352	1.97	0.47
1:B:1650:TYR:HD2	2:B:500:PEV:H31	1.79	0.47
1:A:1633:PHE:HB2	1:A:1668:TYR:OH	2.14	0.47
1:A:1772:LEU:HD21	1:A:1797:GLU:HG3	1.96	0.47
1:A:1629:PRO:HA	1:A:1664:TRP:CZ2	2.50	0.47
1:B:1596:GLN:HB2	1:B:1597:ILE:HG12	1.96	0.47
2:A:400:PEV:H202	2:A:400:PEV:H432	1.97	0.46
1:B:1587:TYR:CE2	1:B:1589:ALA:HA	2.50	0.46
1:A:1660:ASN:HD21	1:A:1759:ASN:ND2	2.13	0.46
1:B:1694:LEU:CD2	1:B:1698:ILE:HD12	2.40	0.46
1:A:1679:LEU:CD2	2:A:400:PEV:H322	2.46	0.46
1:B:1765:SER:HB2	1:B:1810:TRP:CZ2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1646:PRO:O	1:A:1649:ALA:HB3	2.15	0.46
1:B:1587:TYR:HE2	2:B:500:PEV:H212	1.80	0.46
1:B:1695:ALA:HA	1:B:1698:ILE:O	2.16	0.46
2:B:500:PEV:H202	2:B:500:PEV:H432	1.97	0.46
1:B:1602:LEU:HD22	1:B:1602:LEU:C	2.40	0.46
1:B:1662:ASN:HB2	1:B:1760:ASP:OD1	2.16	0.46
1:A:1589:ALA:HB3	1:A:1627:THR:OG1	2.16	0.45
1:A:1607:LEU:CD1	1:A:1645:PHE:HE1	2.26	0.45
1:A:1738:SER:O	1:A:1806:ILE:HG13	2.17	0.45
1:B:1650:TYR:CD2	2:B:500:PEV:C1	2.98	0.45
1:B:1660:ASN:HD22	1:B:1660:ASN:HA	1.53	0.45
1:B:1771:CYS:O	1:B:1778:PHE:HB2	2.16	0.45
1:A:1619:GLU:HG2	1:A:1654:SER:HB3	1.98	0.45
1:B:1789:LEU:HB3	1:B:1791:PHE:HE1	1.79	0.45
1:B:1807:ARG:O	1:B:1810:TRP:HB3	2.17	0.45
1:A:1780:LEU:HD13	1:A:1782:ILE:HD11	1.98	0.45
1:A:1645:PHE:HB2	1:A:1650:TYR:CE1	2.51	0.45
1:A:1604:TYR:CE2	1:A:1608:LEU:HD12	2.51	0.45
1:B:1658:ILE:CD1	1:B:1685:LEU:HD13	2.47	0.45
1:B:1773:VAL:HB	1:B:1777:GLN:HG2	1.98	0.45
1:A:1633:PHE:CZ	2:A:400:PEV:H191	2.52	0.45
1:B:1694:LEU:C	1:B:1696:GLU:H	2.25	0.45
1:B:1601:LEU:HA	1:B:1601:LEU:HD23	1.75	0.45
1:A:1748:ARG:HD3	1:A:1755:SER:O	2.17	0.44
1:B:1651:ASP:HA	1:B:1684:ARG:HH12	1.82	0.44
1:A:1764:ALA:HB2	1:A:1806:ILE:HG23	1.99	0.44
1:A:1646:PRO:HB3	1:A:1648:PHE:CE1	2.52	0.44
1:B:1567:LYS:C	1:B:1569:LEU:N	2.76	0.44
1:B:1597:ILE:O	1:B:1601:LEU:HG	2.17	0.44
1:A:1625:THR:HG23	1:A:1761:ILE:CD1	2.48	0.44
1:A:1720:HIS:O	1:A:1793:HIS:CE1	2.70	0.44
1:A:1809:ARG:HH21	1:B:1809:ARG:NH2	2.15	0.44
1:B:1568:THR:HG23	1:B:1602:LEU:HA	2.00	0.44
1:B:1656:VAL:HB	1:B:1685:LEU:HD22	2.00	0.44
1:B:1701:GLU:OE1	1:B:1701:GLU:HA	2.16	0.44
1:A:1594:THR:HG23	1:A:1630:SER:O	2.18	0.43
1:B:1625:THR:HG22	1:B:1660:ASN:OD1	2.17	0.43
1:A:1607:LEU:HD12	1:A:1645:PHE:CE1	2.49	0.43
1:A:1685:LEU:HB2	1:A:1754:GLN:NE2	2.33	0.43
1:B:1616:LYS:HB3	1:B:1617:PRO:HD2	1.98	0.43
1:B:1793:HIS:HD2	1:B:1795:GLU:N	2.12	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:ASN:ND2	1:A:1665:VAL:HG23	2.21	0.43
1:A:1685:LEU:HB2	1:A:1754:GLN:HE22	1.83	0.43
1:B:1596:GLN:HB2	1:B:1597:ILE:H	1.30	0.43
1:B:1602:LEU:HD22	1:B:1606:VAL:HG23	1.99	0.43
1:A:1611:LYS:HA	1:A:1614:TYR:CE2	2.54	0.43
1:B:1762:TYR:CZ	1:B:1789:LEU:HD21	2.54	0.43
1:A:1633:PHE:CE1	2:A:400:PEV:H191	2.53	0.43
1:A:1624:LEU:HD23	1:A:1624:LEU:HA	1.88	0.43
1:A:1720:HIS:O	1:A:1793:HIS:HE1	2.02	0.43
1:A:1584:ILE:CD1	1:A:1698:ILE:HG12	2.49	0.43
1:A:1606:VAL:HG21	1:A:1641:TRP:HH2	1.84	0.43
1:B:1690:CYS:HA	1:B:1691:PRO:HD2	1.70	0.43
1:B:1779:THR:HA	1:B:1789:LEU:O	2.18	0.43
1:A:1595:GLY:O	1:A:1596:GLN:CB	2.67	0.42
1:B:1617:PRO:HA	1:B:1652:ASN:O	2.19	0.42
1:A:1579:LYS:HG3	1:A:1698:ILE:O	2.20	0.42
1:A:1611:LYS:CB	1:A:1612:PRO:CD	2.80	0.42
1:A:1793:HIS:HD2	1:A:1795:GLU:H	1.62	0.42
1:A:1800:VAL:O	1:A:1804:ILE:HG13	2.19	0.42
1:B:1620:ILE:O	1:B:1656:VAL:HA	2.19	0.42
1:B:1650:TYR:HD2	2:B:500:PEV:C1	2.28	0.42
1:B:1665:VAL:O	1:B:1669:THR:HG23	2.19	0.42
1:B:1782:ILE:CG1	1:B:1789:LEU:HD22	2.50	0.42
1:A:1695:ALA:HB1	1:A:1701:GLU:HB3	2.01	0.42
1:A:1610:LEU:O	1:A:1611:LYS:C	2.62	0.42
1:A:1716:LEU:HD23	1:A:1735:LYS:HD3	2.01	0.42
2:A:400:PEV:H182	2:A:400:PEV:H452	2.02	0.42
1:B:1657:TYR:HA	1:B:1686:VAL:O	2.19	0.42
1:A:1611:LYS:CB	1:A:1612:PRO:HD2	2.48	0.41
2:B:500:PEV:H182	2:B:500:PEV:H452	2.02	0.41
1:A:1684:ARG:H	1:A:1684:ARG:HG3	1.57	0.41
1:A:1711:ALA:O	1:A:1714:GLU:HG2	2.19	0.41
1:B:1575:ALA:HB1	1:B:1704:LYS:HG3	2.02	0.41
1:B:1694:LEU:HD22	1:B:1703:GLN:CD	2.45	0.41
1:A:1653:VAL:HB	1:A:1684:ARG:NH2	2.35	0.41
1:B:1568:THR:CG2	1:B:1602:LEU:HA	2.51	0.41
1:A:1695:ALA:HB1	1:A:1701:GLU:CA	2.51	0.41
1:B:1597:ILE:HD13	1:B:1597:ILE:HG23	1.88	0.41
1:A:1572:PHE:HA	1:A:1586:TYR:O	2.21	0.41
1:A:1622:VAL:HG13	1:A:1658:ILE:HA	2.02	0.41
2:B:500:PEV:H411	2:B:500:PEV:C20	2.50	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1780:LEU:HD21	1:A:1803:ILE:HG21	2.02	0.41
1:A:1769:GLU:HB2	1:A:1781:THR:HB	2.03	0.41
2:A:400:PEV:H411	2:A:400:PEV:C20	2.50	0.41
1:B:1572:PHE:CG	1:B:1606:VAL:HG22	2.56	0.41
1:B:1694:LEU:HD23	1:B:1694:LEU:C	2.46	0.41
1:A:1660:ASN:HD22	1:A:1660:ASN:HA	1.51	0.41
1:B:1624:LEU:HD13	1:B:1665:VAL:HG11	2.03	0.41
1:B:1679:LEU:HD11	2:B:500:PEV:H322	2.04	0.40
1:A:1618:TYR:HE1	1:A:1620:ILE:HD11	1.86	0.40
1:A:1607:LEU:HD12	1:A:1607:LEU:HA	1.72	0.40
1:A:1665:VAL:CG1	2:A:400:PEV:H391	2.52	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	248/277 (90%)	232 (94%)	11 (4%)	5 (2%)	6	10
1	B	248/277 (90%)	229 (92%)	15 (6%)	4 (2%)	7	14
All	All	496/554 (90%)	461 (93%)	26 (5%)	9 (2%)	6	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1597	ILE
1	B	1596	GLN
1	B	1691	PRO
1	A	1596	GLN
1	A	1699	GLU
1	B	1614	TYR
1	A	1786	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1813	SER
1	A	1643	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	218/244 (89%)	192 (88%)	26 (12%)	5 11
1	B	219/244 (90%)	189 (86%)	30 (14%)	3 7
All	All	437/488 (90%)	381 (87%)	56 (13%)	4 9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1578	SER
1	A	1590	ARG
1	A	1591	ARG
1	A	1593	LYS
1	A	1594	THR
1	A	1596	GLN
1	A	1601	LEU
1	A	1602	LEU
1	A	1608	LEU
1	A	1614	TYR
1	A	1616	LYS
1	A	1620	ILE
1	A	1622	VAL
1	A	1634	LYS
1	A	1643	VAL
1	A	1644	VAL
1	A	1660	ASN
1	A	1662	ASN
1	A	1669	THR
1	A	1674	ARG
1	A	1725	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1755	SER
1	A	1779	THR
1	A	1780	LEU
1	A	1806	ILE
1	A	1809	ARG
1	B	1568	THR
1	B	1594	THR
1	B	1596	GLN
1	B	1597	ILE
1	B	1600	ASP
1	B	1602	LEU
1	B	1614	TYR
1	B	1638	LEU
1	B	1646	PRO
1	B	1660	ASN
1	B	1670	LYS
1	B	1673	GLU
1	B	1683	LYS
1	B	1710	LEU
1	B	1723	LEU
1	B	1730	THR
1	B	1743	VAL
1	B	1749	THR
1	B	1756	VAL
1	B	1775	GLU
1	B	1776	ASN
1	B	1779	THR
1	B	1780	LEU
1	B	1787	THR
1	B	1789	LEU
1	B	1790	THR
1	B	1801	GLN
1	B	1802	SER
1	B	1807	ARG
1	B	1814	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1596	GLN
1	A	1660	ASN
1	A	1662	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1672	HIS
1	A	1754	GLN
1	A	1784	ASN
1	A	1785	GLN
1	A	1793	HIS
1	A	1794	GLN
1	A	1801	GLN
1	A	1805	HIS
1	A	1814	GLN
1	B	1582	ASN
1	B	1660	ASN
1	B	1672	HIS
1	B	1754	GLN
1	B	1759	ASN
1	B	1777	GLN
1	B	1785	GLN
1	B	1793	HIS
1	B	1801	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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$
2	PEV	B	500	-	48,48,48	0.53	0	51,53,53	1.26	4 (7%)
2	PEV	A	400	-	48,48,48	0.54	0	51,53,53	1.26	4 (7%)
3	POP	B	601	-	6,8,8	0.92	0	12,13,13	0.97	1 (8%)
3	POP	B	602	-	6,8,8	1.18	0	12,13,13	1.07	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
2	PEV	B	500	-	1/1/4/4	7/52/52/52	-
2	PEV	A	400	-	1/1/4/4	7/52/52/52	-
3	POP	B	601	-	-	1/6/6/6	-
3	POP	B	602	-	-	1/6/6/6	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PEV	C26-C25-C24	5.54	150.79	113.36
2	A	400	PEV	C26-C25-C24	5.54	150.77	113.36
2	B	500	PEV	O2-C31-C32	3.18	118.35	111.48
2	A	400	PEV	O2-C31-C32	3.16	118.32	111.48
2	B	500	PEV	C3-C2-C1	-2.77	105.32	111.78
2	A	400	PEV	C3-C2-C1	-2.77	105.33	111.78
2	B	500	PEV	O3-C11-C12	2.64	119.87	111.83
2	A	400	PEV	O3-C11-C12	2.62	119.83	111.83
3	B	601	POP	O2-P1-O	2.03	111.44	104.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	400	PEV	C2
2	B	500	PEV	C2

All (16) torsion outliers are listed below:

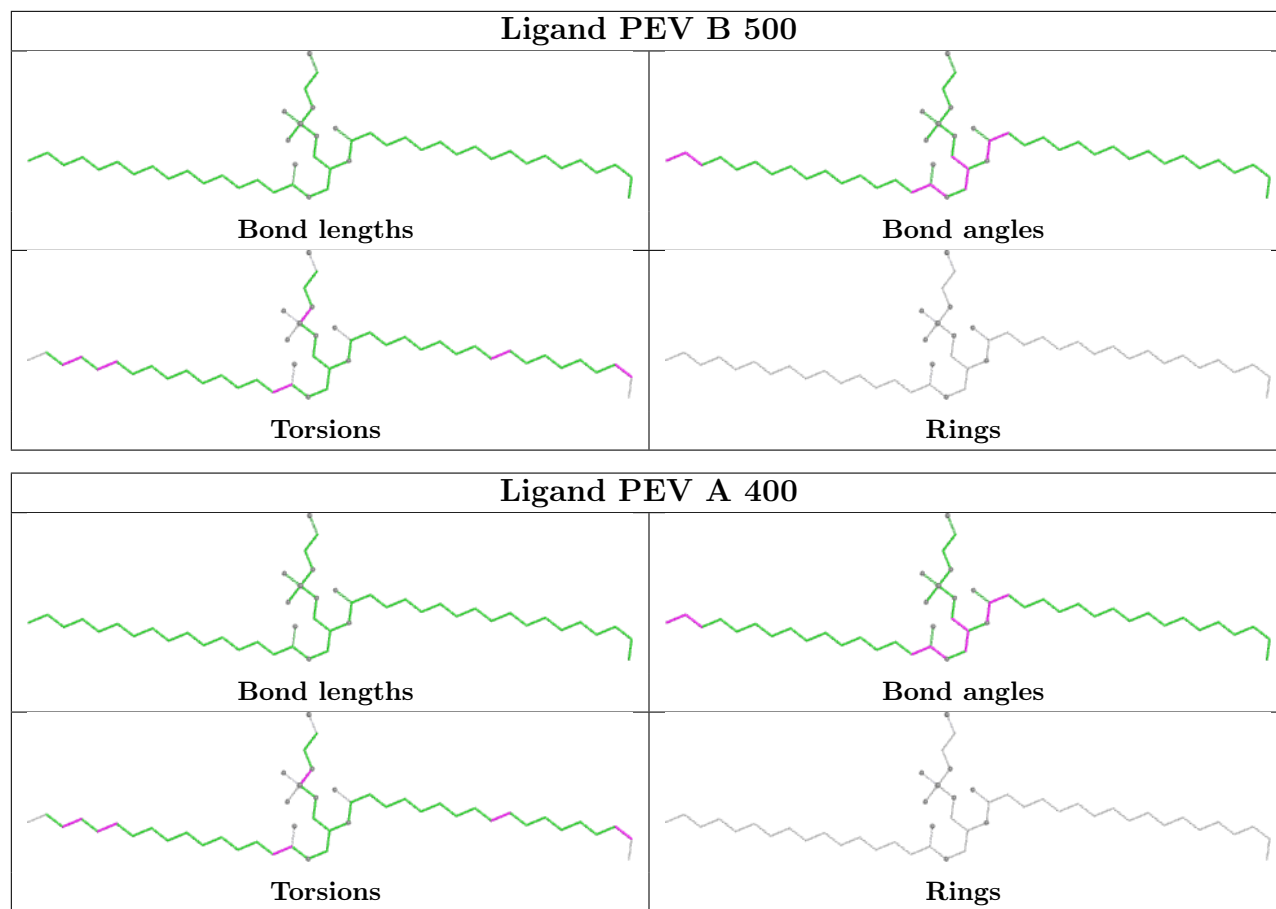
Mol	Chain	Res	Type	Atoms
3	B	602	POP	P2-O-P1-O3
2	A	400	PEV	C22-C23-C24-C25
2	B	500	PEV	C22-C23-C24-C25
2	A	400	PEV	C45-C46-C47-C48
2	B	500	PEV	C45-C46-C47-C48
3	B	601	POP	P1-O-P2-O4
2	A	400	PEV	C4-O4P-P-O1P
2	B	500	PEV	C4-O4P-P-O1P
2	B	500	PEV	C38-C39-C40-C41
2	A	400	PEV	C38-C39-C40-C41
2	A	400	PEV	C20-C21-C22-C23
2	B	500	PEV	C20-C21-C22-C23
2	A	400	PEV	O3-C11-C12-C13
2	B	500	PEV	O3-C11-C12-C13
2	A	400	PEV	O11-C11-C12-C13
2	B	500	PEV	O11-C11-C12-C13

There are no ring outliers.

3 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	PEV	49	0
2	A	400	PEV	17	0
3	B	602	POP	2	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, 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	250/277 (90%)	0.65	16 (6%) 25 22	33, 57, 84, 95	0
1	B	250/277 (90%)	0.46	10 (4%) 42 38	25, 50, 71, 79	0
All	All	500/554 (90%)	0.55	26 (5%) 33 29	25, 53, 79, 95	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1595	GLY	6.5
1	A	1597	ILE	5.7
1	A	1594	THR	4.5
1	B	1595	GLY	4.2
1	A	1700	HIS	4.2
1	A	1673	GLU	3.4
1	A	1701	GLU	3.4
1	B	1596	GLN	3.1
1	A	1596	GLN	3.0
1	A	1567	LYS	2.9
1	A	1695	ALA	2.9
1	A	1604	TYR	2.8
1	B	1597	ILE	2.8
1	A	1699	GLU	2.8
1	A	1579	LYS	2.6
1	B	1568	THR	2.6
1	A	1696	GLU	2.4
1	B	1598	ASN	2.4
1	B	1680	LYS	2.3
1	A	1568	THR	2.3
1	B	1691	PRO	2.3
1	A	1776	ASN	2.2
1	B	1727	HIS	2.2
1	A	1602	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	1569	LEU	2.1
1	B	1771	CYS	2.1

## 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](#)

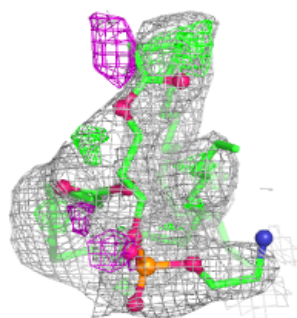
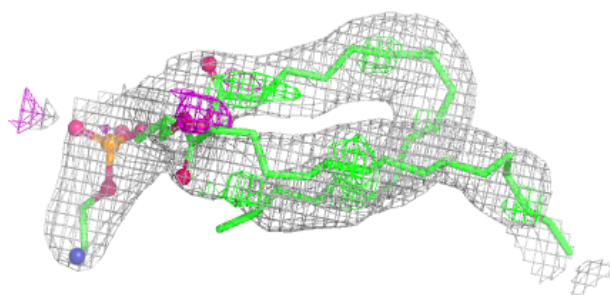
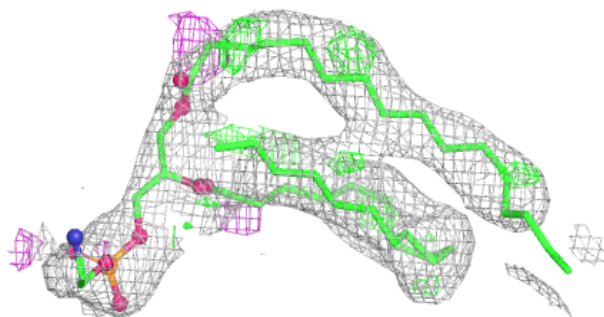
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	POP	B	601	9/9	0.54	0.19	145,147,151,151	0
2	PEV	B	500	49/49	0.72	0.20	20,71,84,86	3
2	PEV	A	400	49/49	0.74	0.18	20,71,84,86	3
3	POP	B	602	9/9	0.87	0.22	83,94,101,104	0

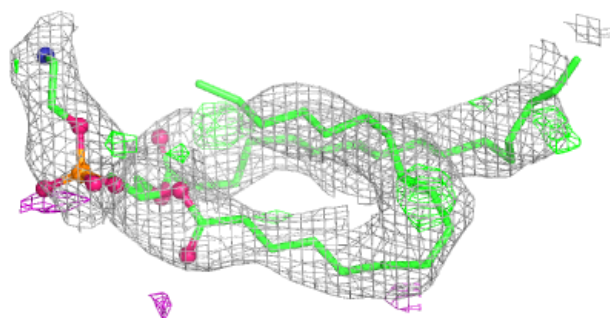
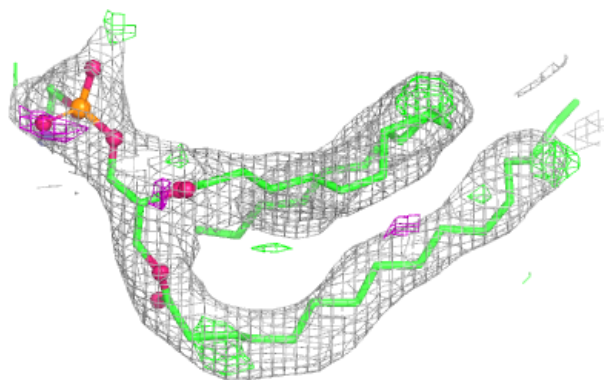
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PEV 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 PEV 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

There are no such residues in this entry.