



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 AM GMT

PDB ID : 2E2X
Title : Sec14 Homology Module of Neurofibromin in complex with phosphatidylethanolamine
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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

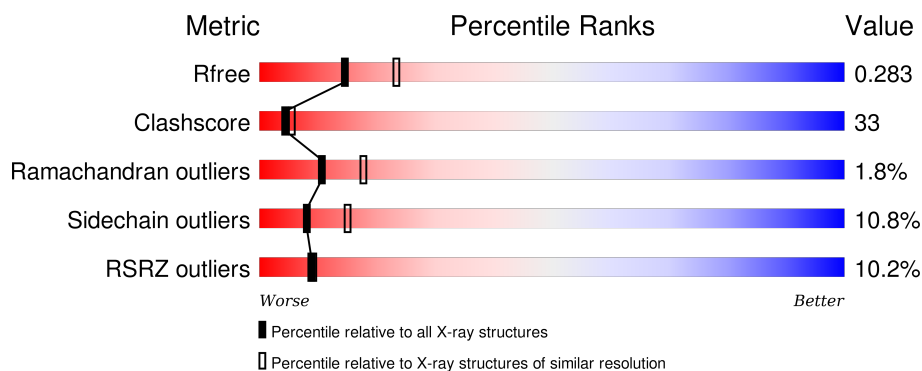
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>9%</div> <div>46%</div> <div>38%</div> <div>7%</div> <div>10%</div> </div>
1	B	277	<div> <div>9%</div> <div>45%</div> <div>40%</div> <div>• •</div> <div>10%</div> </div>

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	-	-	X
2	PEV	B	500	X	-	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.

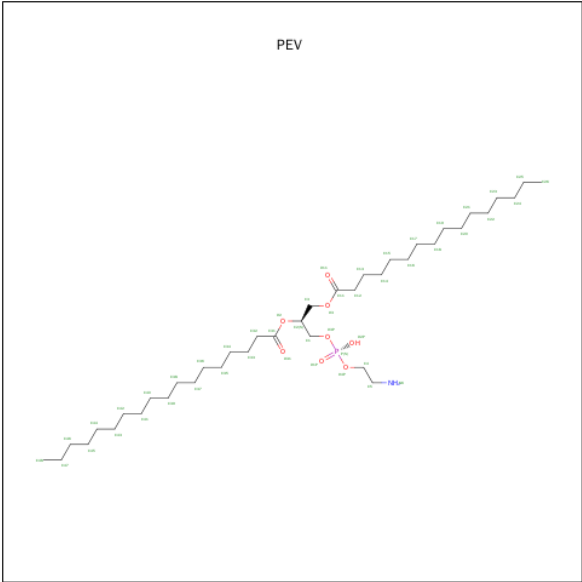
- Molecule 1 is a protein called Neurofibromin.

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

There are 10 discrepancies between the modelled and reference sequences:

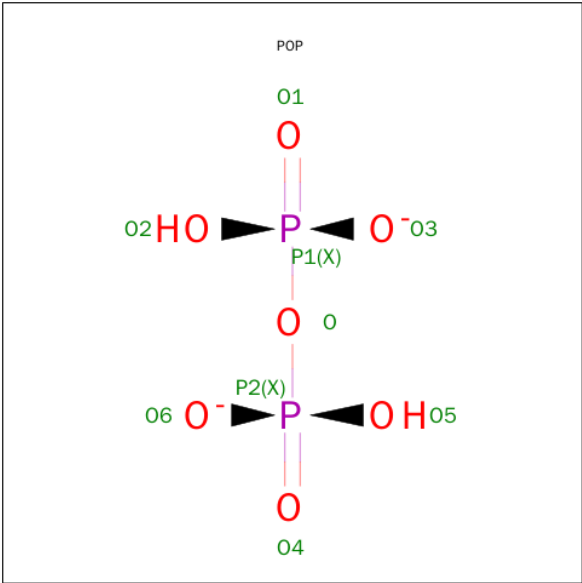
Chain	Residue	Modelled	Actual	Comment	Reference
A	1540	GLY	-	EXPRESSION TAG	UNP P21359
A	1541	ALA	-	EXPRESSION TAG	UNP P21359
A	1542	MET	-	EXPRESSION TAG	UNP P21359
A	1543	THR	-	EXPRESSION TAG	UNP P21359
A	1544	GLY	-	EXPRESSION TAG	UNP P21359
B	1540	GLY	-	EXPRESSION TAG	UNP P21359
B	1541	ALA	-	EXPRESSION 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-{|(PALMITOYLOXY)METHYL|ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P).



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- (three-letter code: 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		

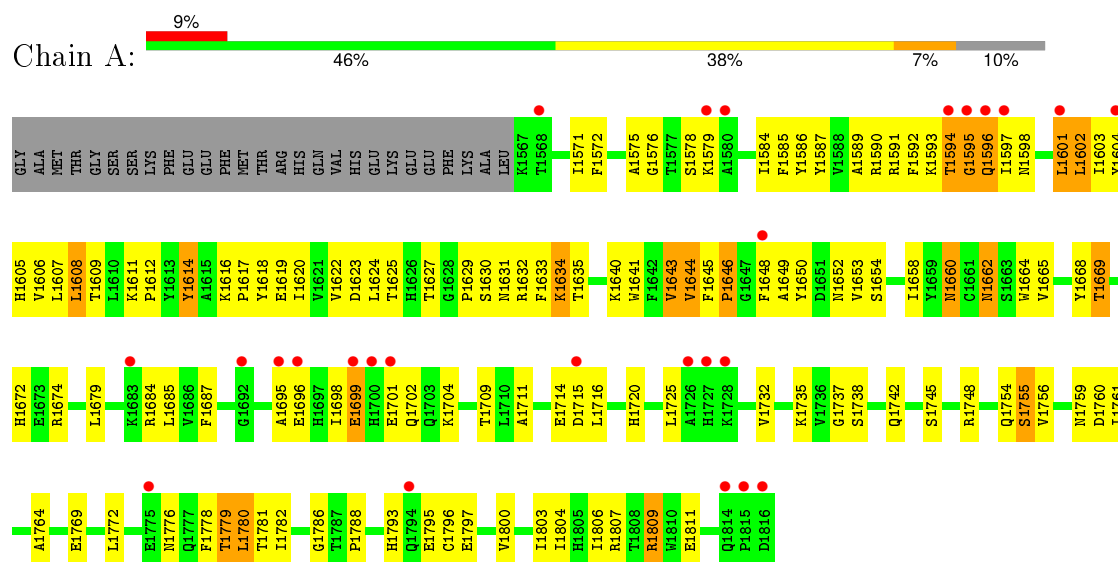
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	44	Total 44	O 44	0	0

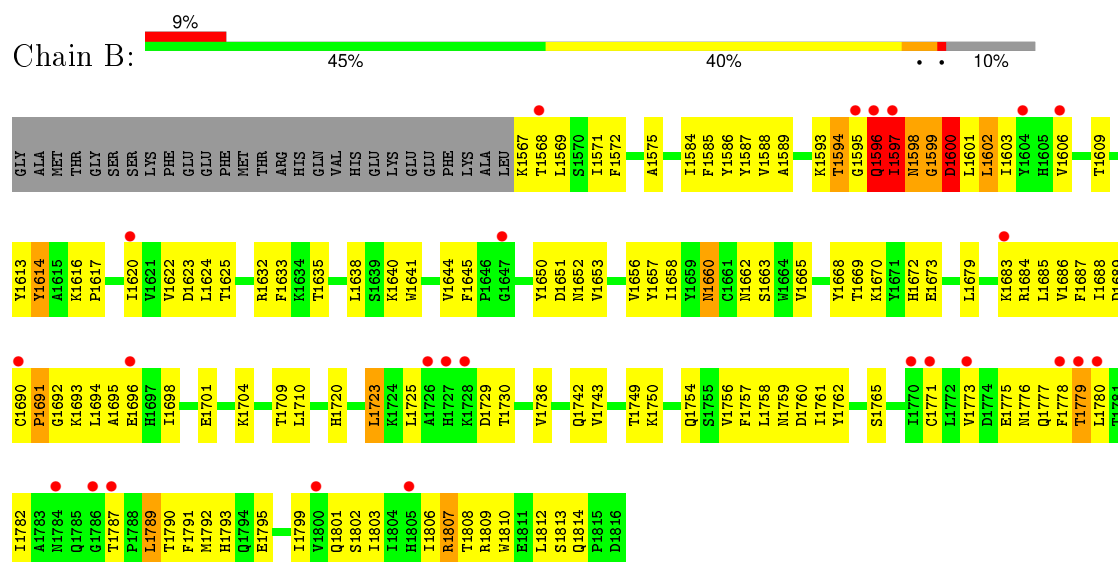
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	110.10Å 110.10Å 121.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 19.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 99.6 (19.46-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.254 , 0.283 0.266 , 0.283	Depositor DCC
R_{free} test set	1286 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 49309 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4218	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.49	0/2063	0.75	2/2801 (0.1%)
1	B	0.60	1/2065 (0.0%)	0.89	5/2804 (0.2%)
All	All	0.55	1/4128 (0.0%)	0.82	7/5605 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1596	GLN	CG-CD	6.31	1.65	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1599	GLY	C-N-CA	-8.78	99.76	121.70
1	B	1595	GLY	CA-C-N	-6.49	102.91	117.20
1	A	1595	GLY	N-CA-C	-5.88	98.40	113.10
1	A	1646	PRO	N-CA-C	-5.59	97.57	112.10
1	B	1597	ILE	C-N-CA	-5.40	108.20	121.70
1	B	1598	ASN	C-N-CA	-5.33	111.12	122.30
1	B	1600	ASP	CB-CG-OD1	5.12	122.91	118.30

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	2013	0	1994	118	0
1	B	2015	0	1999	138	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	271	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 (271) 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
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:B:1679:LEU:HD21	2:B:500:PEV:C32	2.10	0.79
1:A:1594:THR:HG21	1:A:1632:ARG:HG2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1742:GLN:HG2	1:B:1761:ILE:HG12	1.63	0.79
1:B:1679:LEU:CD2	2:B:500:PEV:C32	2.63	0.77
1:B:1650:TYR:CD2	2:B:500:PEV:H12	2.20	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
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:B:1689:ASP:HB3	1:B:1757:PHE:HD2	1.59	0.66
1:A:1617:PRO:HA	1:A:1652:ASN:HB3	1.77	0.66
1:B:1620:ILE:HD12	2:B:500:PEV:C12	2.13	0.65
1:A:1614:TYR:CZ	1:A:1646:PRO:HG2	2.32	0.65
1:A:1587:TYR:CD2	2:A:400:PEV:H192	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1633:PHE:CZ	2:B:500:PEV:H191	2.33	0.63
1:A:1650:TYR:HD2	2:A:400:PEV:H12	1.63	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:B:1602:LEU:HD13	1:B:1641:TRP:HZ2	1.63	0.62
1:A:1587:TYR:HE1	1:A:1602:LEU:HD11	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: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:H412	2:B:500:PEV:H371	1.86	0.57
1:A:1779:THR:HG23	1:A:1788:PRO:HB2	1.86	0.57
1:B:1679:LEU:CD2	2:B:500:PEV:C31	2.82	0.57
2:A:400:PEV:H371	2:A:400:PEV:H412	1.86	0.57
1:A:1650:TYR:CD2	2:A:400:PEV:H12	2.39	0.57
1:B:1687:PHE:CG	1:B:1756:VAL:HG11	2.39	0.57
1:B:1568:THR:HA	1:B:1571:ILE:HD12	1.87	0.57
1:A:1644:VAL:O	1:A:1644:VAL:HG13	2.04	0.57
1:B:1620:ILE:HD11	2:B:500:PEV:C13	2.16	0.57
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:O	1:A:1643:VAL:HG13	2.05	0.56
1:B:1690:CYS:C	1:B:1692:GLY:H	2.08	0.56
1:B:1742:GLN:HB3	1:B:1759:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H411	2:B:500:PEV:H202	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:B:1650:TYR:HA	2:B:500:PEV:H32	1.89	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:1625:THR:HG22	1:B:1660:ASN:HB2	1.91	0.53
1:B:1690:CYS:C	1:B:1692:GLY:N	2.61	0.52
1:B:1736:VAL:HG13	1:B:1806:ILE:HD13	1.90	0.52
1:B:1635:THR:OG1	1:B:1672:HIS:HE1	1.92	0.52
2:A:400:PEV:H441	2:A:400:PEV:H341	1.92	0.52
1:A:1643:VAL:CG1	1:A:1643:VAL:O	2.56	0.52
1:A:1702:GLN:HG3	1:A:1704:LYS:HE2	1.91	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: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
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
2:B:500:PEV:H441	2:B:500:PEV:H341	1.92	0.50
1:B:1658:ILE:HD11	1:B:1685:LEU:HD13	1.92	0.50
1:A:1598:ASN:O	1:A:1601:LEU:HB2	2.12	0.50
1:A:1776:ASN:HA	1:A:1796:CYS:HB2	1.93	0.50
1:B:1641:TRP:HB3	2:B:500:PEV:H471	1.94	0.50
1:B:1585:PHE:HZ	1:B:1613:TYR:CD1	2.29	0.50
1:B:1587:TYR:HH	1:B:1633:PHE:HE2	1.56	0.49
1:B:1688:ILE:HG21	1:B:1694:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1750:LYS:HA	1:B:1754:GLN:O	2.13	0.49
1:B:1663:SER:HA	1:B:1758:LEU:HD13	1.95	0.49
1:B:1587:TYR:CE2	2:B:500:PEV:H212	2.48	0.49
1:B:1584:ILE:HD13	1:B:1698:ILE:HD13	1.94	0.49
1:A:1742:GLN:HG2	1:A:1761:ILE:HG12	1.95	0.49
1:A:1589:ALA:O	1:A:1631:ASN:HB3	2.13	0.49
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:B:1597:ILE:O	1:B:1598:ASN:C	2.52	0.47
1:B:1650:TYR:CD1	2:B:500:PEV:N6	2.83	0.47
1:B:1625:THR:HG22	1:B:1660:ASN:CB	2.45	0.47
1:A:1778:PHE:HE1	1:A:1780:LEU:HG	1.78	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:B:1596:GLN:HB2	1:B:1597:ILE:HG12	1.96	0.47
1:A:1629:PRO:HA	1:A:1664:TRP:CZ2	2.50	0.47
1:B:1587:TYR:CE2	1:B:1589:ALA:HA	2.50	0.46
2:A:400:PEV:H432	2:A:400:PEV:H202	1.97	0.46
1:B:1694:LEU:CD2	1:B:1698:ILE:HD12	2.40	0.46
1:A:1660:ASN:HD21	1:A:1759:ASN:ND2	2.13	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
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
2:B:500:PEV:H432	2:B:500:PEV:H202	1.97	0.46
1:B:1695:ALA:HA	1:B:1698:ILE:O	2.16	0.46
1:A:1662:ASN:HD22	1:A:1662:ASN:C	2.17	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:HA	1:B:1660:ASN:HD22	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1771:CYS:O	1:B:1778:PHE:HB2	2.16	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:1619:GLU:HG2	1:A:1654:SER:HB3	1.98	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: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:1604:TYR:CE2	1:A:1608:LEU:HD12	2.51	0.45
1:A:1633:PHE:CZ	2:A:400:PEV:H191	2.52	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: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:1567:LYS:C	1:B:1569:LEU:H	2.21	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:B:1793:HIS:HD2	1:B:1795:GLU:N	2.12	0.43
1:B:1616:LYS:HB3	1:B:1617:PRO:HD2	1.98	0.43
1:A:1685:LEU:HB2	1:A:1754:GLN:NE2	2.33	0.43
1:B:1602:LEU:HD22	1:B:1606:VAL:HG23	1.99	0.43
1:B:1596:GLN:HB2	1:B:1597:ILE:H	1.30	0.43
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: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:HA	1:A:1624:LEU:HD23	1.88	0.43
1:A:1720:HIS:O	1:A:1793:HIS:HE1	2.02	0.43
1:B:1690:CYS:HA	1:B:1691:PRO:HD2	1.70	0.43
1:A:1606:VAL:HG21	1:A:1641:TRP:HH2	1.84	0.43
1:B:1779:THR:HA	1:B:1789:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1584:ILE:CD1	1:A:1698:ILE:HG12	2.49	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:1611:LYS:CB	1:A:1612:PRO:CD	2.80	0.42
1:A:1579:LYS:HG3	1:A:1698:ILE:O	2.20	0.42
1:B:1650:TYR:HD2	2:B:500:PEV:C1	2.28	0.42
1:B:1620:ILE:O	1:B:1656:VAL:HA	2.19	0.42
1:A:1793:HIS:HD2	1:A:1795:GLU:H	1.62	0.42
1:B:1782:ILE:CG1	1:B:1789:LEU:HD22	2.50	0.42
1:A:1800:VAL:O	1:A:1804:ILE:HG13	2.19	0.42
1:B:1665:VAL:O	1:B:1669:THR:HG23	2.19	0.42
1:A:1695:ALA:HB1	1:A:1701:GLU:HB3	2.01	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:H452	2:B:500:PEV:H182	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:1568:THR:CG2	1:B:1602:LEU:HA	2.51	0.41
1:A:1653:VAL:HB	1:A:1684:ARG:NH2	2.35	0.41
1:B:1597:ILE:HG23	1:B:1597:ILE:HD13	1.88	0.41
1:A:1695:ALA:HB1	1:A:1701:GLU:CA	2.51	0.41
1:B:1602:LEU:HD22	1:B:1602:LEU:C	2.40	0.41
2:B:500:PEV:H411	2:B:500:PEV:C20	2.50	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
1:A:1780:LEU:HD21	1:A:1803:ILE:HG21	2.02	0.41
1:B:1572:PHE:CG	1:B:1606:VAL:HG22	2.56	0.41
2:A:400:PEV:H411	2:A:400:PEV:C20	2.50	0.41
1:A:1769:GLU:HB2	1:A:1781:THR:HB	2.03	0.41
1:A:1660:ASN:HA	1:A:1660:ASN:HD22	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:HA	1:A:1607:LEU:HD12	1.72	0.40
1:A:1665:VAL:CG1	2:A:400:PEV:H391	2.52	0.40
1:B:1694:LEU:C	1:B:1696:GLU:H	2.25	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%)	9	15
1	B	248/277 (90%)	229 (92%)	15 (6%)	4 (2%)	12	21
All	All	496/554 (90%)	461 (93%)	26 (5%)	9 (2%)	11	18

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
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%)	197 (90%)	21 (10%)	10	19
1	B	219/244 (90%)	193 (88%)	26 (12%)	6	12
All	All	437/488 (90%)	390 (89%)	47 (11%)	8	15

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1578	SER
1	A	1591	ARG
1	A	1593	LYS
1	A	1594	THR
1	A	1601	LEU
1	A	1602	LEU
1	A	1608	LEU
1	A	1614	TYR
1	A	1616	LYS
1	A	1634	LYS
1	A	1644	VAL
1	A	1660	ASN
1	A	1662	ASN
1	A	1669	THR
1	A	1674	ARG
1	A	1715	ASP
1	A	1725	LEU
1	A	1755	SER
1	A	1779	THR
1	A	1780	LEU
1	A	1809	ARG
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	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	1749	THR
1	B	1775	GLU
1	B	1776	ASN
1	B	1779	THR
1	B	1780	LEU
1	B	1787	THR
1	B	1789	LEU

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Mol	Chain	Res	Type
1	B	1790	THR
1	B	1801	GLN
1	B	1802	SER
1	B	1807	ARG
1	B	1814	GLN

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

Mol	Chain	Res	Type
1	A	1596	GLN
1	A	1660	ASN
1	A	1662	ASN
1	A	1672	HIS
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	1660	ASN
1	B	1672	HIS
1	B	1703	GLN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	400	-	47,48,48	0.53	0	48,53,53	1.23	4 (8%)
2	PEV	B	500	-	47,48,48	0.53	0	48,53,53	1.23	4 (8%)
3	POP	B	601	-	8,8,8	0.59	0	13,13,13	1.86	1 (7%)
3	POP	B	602	-	8,8,8	0.84	0	13,13,13	1.86	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
2	PEV	A	400	-	1/1/4/4	0/52/52/52	0/0/0/0
2	PEV	B	500	-	1/1/4/4	0/52/52/52	0/0/0/0
3	POP	B	601	-	-	0/6/6/6	0/0/0/0
3	POP	B	602	-	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	POP	P2-O-P1	-6.06	115.71	132.73
3	B	602	POP	P2-O-P1	-5.99	115.89	132.73
2	B	500	PEV	C3-C2-C1	-2.88	105.32	112.07
2	A	400	PEV	C3-C2-C1	-2.88	105.33	112.07
2	A	400	PEV	O3-C11-C12	2.60	119.83	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PEV	O3-C11-C12	2.62	119.87	111.90
2	A	400	PEV	O2-C31-C32	3.13	118.32	111.53
2	B	500	PEV	O2-C31-C32	3.14	118.35	111.53
2	A	400	PEV	C26-C25-C24	4.75	150.77	113.44
2	B	500	PEV	C26-C25-C24	4.75	150.79	113.44

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	PEV	17	0
2	B	500	PEV	49	0
3	B	602	POP	2	0

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	250/277 (90%)	0.70	26 (10%) 8 8	33, 57, 84, 95	0
1	B	250/277 (90%)	0.61	25 (10%) 9 10	25, 50, 71, 79	0
All	All	500/554 (90%)	0.66	51 (10%) 9 9	25, 53, 79, 95	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1595	GLY	11.2
1	A	1596	GLN	7.0
1	A	1604	TYR	5.2
1	A	1700	HIS	4.7
1	A	1815	PRO	4.6
1	B	1770	ILE	4.1
1	B	1771	CYS	4.1
1	B	1727	HIS	4.1
1	B	1597	ILE	3.9
1	A	1597	ILE	3.8
1	B	1604	TYR	3.8
1	A	1579	LYS	3.6
1	A	1727	HIS	3.5
1	A	1594	THR	3.4
1	B	1595	GLY	3.2
1	A	1696	GLU	3.1
1	B	1690	CYS	3.0
1	A	1816	ASP	2.9
1	B	1786	GLY	2.9
1	A	1814	GLN	2.8
1	A	1701	GLU	2.8
1	B	1596	GLN	2.7
1	B	1784	ASN	2.7
1	B	1696	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1620	ILE	2.7
1	A	1683	LYS	2.7
1	B	1568	THR	2.6
1	A	1580	ALA	2.6
1	B	1778	PHE	2.6
1	A	1692	GLY	2.5
1	A	1715	ASP	2.5
1	B	1805	HIS	2.5
1	A	1726	ALA	2.5
1	B	1683	LYS	2.4
1	A	1699	GLU	2.4
1	B	1728	LYS	2.3
1	A	1728	LYS	2.3
1	B	1726	ALA	2.3
1	B	1800	VAL	2.3
1	A	1794	GLN	2.3
1	B	1779	THR	2.3
1	B	1787	THR	2.3
1	A	1601	LEU	2.2
1	A	1695	ALA	2.2
1	A	1568	THR	2.2
1	A	1775	GLU	2.2
1	A	1648	PHE	2.1
1	B	1606	VAL	2.0
1	B	1773	VAL	2.0
1	B	1647	GLY	2.0
1	B	1780	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(\AA^2)	Q<0.9
2	PEV	B	500	49/49	0.67	0.42	4.48	20,71,84,86	3
2	PEV	A	400	49/49	0.73	0.38	4.47	20,71,84,86	3
3	POP	B	602	9/9	0.91	0.27	1.72	83,94,101,104	0
3	POP	B	601	9/9	0.66	0.20	-0.20	145,147,151,151	0

6.5 Other polymers

There are no such residues in this entry.