



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:18 PM GMT

PDB ID : 2E2X  
Title : Sec14 Homology Module of Neurofibromin in complex with phosphatidylinositol  
Authors : D'Angelo, I.; Welte, S.; Scheffzek, K.  
Deposited on : 2006-11-18  
Resolution : 2.50 Å (reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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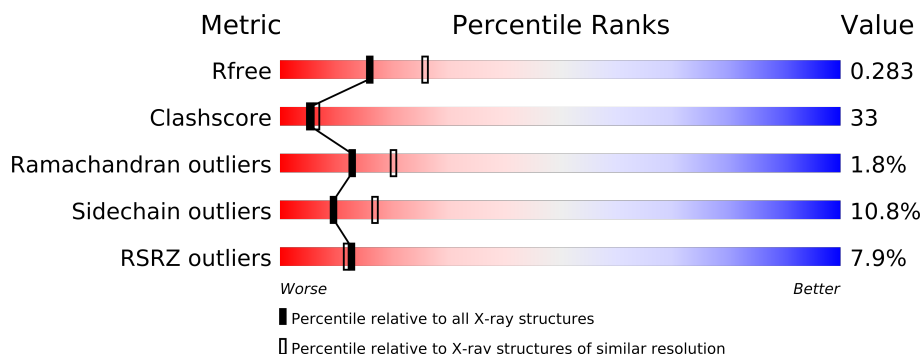
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

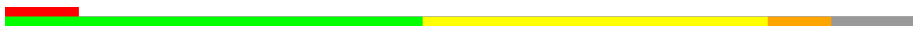
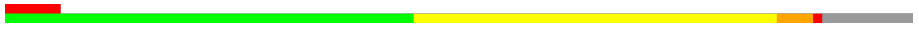
The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	277	
1	B	277	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PEV	A	400	-	X
2	PEV	B	500	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4218 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

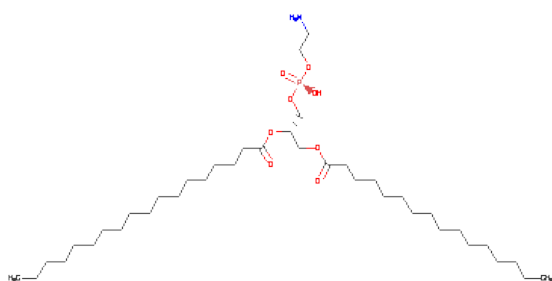
- Molecule 1 is a protein called Neurofibromin.

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:

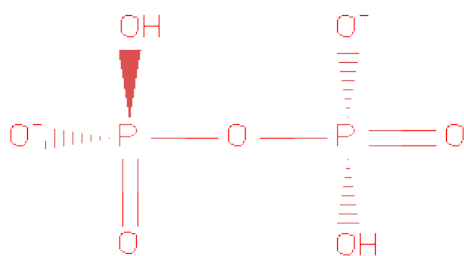
Chain	Residue	Modelled	Actual	Comment	Reference
A	1540	GLY	-	EXPRESSION TAG	UNP P21359
A	1541	ALA	-	EXPRESSION TAG	UNP P21359
A	1542	MET	-	EXPRESSION TAG	UNP P21359
A	1543	THR	-	EXPRESSION TAG	UNP P21359
A	1544	GLY	-	EXPRESSION TAG	UNP P21359
B	1540	GLY	-	EXPRESSION TAG	UNP P21359
B	1541	ALA	-	EXPRESSION 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]ETHYLSTEARATE (three-letter code: 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- (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.

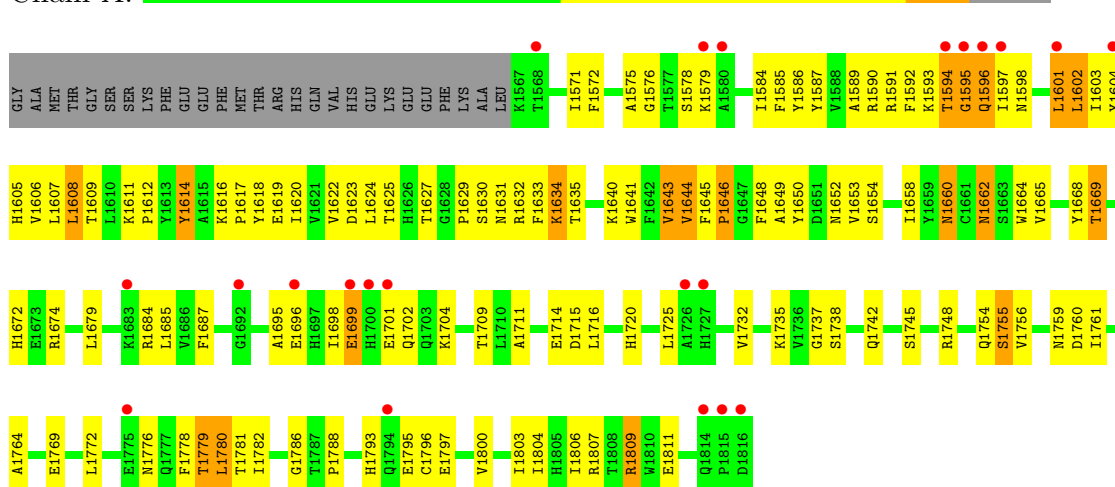
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	44	Total 44	O 44	0	0

### 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.

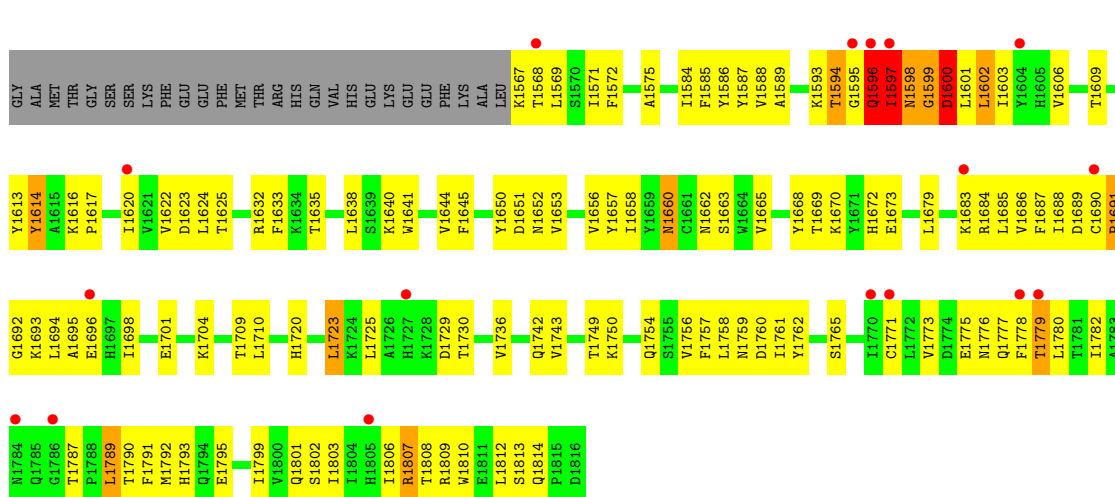
#### • Molecule 1: Neurofibromin

Chain A:



#### • Molecule 1: Neurofibromin

Chain B:



## 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 19.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 99.5 (19.46-2.50)	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)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.254 , 0.283 0.268 , 0.283	Depositor DCC
$R_{free}$ test set	1293 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 26.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the



chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (271) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1594:THR:HG21	1:A:1632:ARG:HG2	1.62	0.79
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	Distance(Å)	Clash(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
2:A:400:PEV:H202	2:A:400:PEV:H411	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

### 5.3.1 Protein backbone ⓘ

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%)	11	17
1	B	248/277 (90%)	229 (92%)	15 (6%)	4 (2%)	14	23
All	All	496/554 (90%)	461 (93%)	26 (5%)	9 (2%)	13	20

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 ⓘ

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%)	12	22
1	B	219/244 (90%)	193 (88%)	26 (12%)	8	13
All	All	437/488 (90%)	390 (89%)	47 (11%)	9	17

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
1	B	1790	THR

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Mol	Chain	Res	Type
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 chains 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	-	48,48,48	0.54	0	53,53,53	1.14	4 (7%)
2	PEV	B	500	-	48,48,48	0.54	0	53,53,53	1.14	4 (7%)
3	POP	B	601	-	8,8,8	0.56	0	13,13,13	1.77	2 (15%)
3	POP	B	602	-	8,8,8	0.81	0	13,13,13	1.79	2 (15%)

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 (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	POP	P2-O-P1	-5.33	115.71	131.74
3	B	602	POP	P2-O-P1	-5.27	115.89	131.74
2	B	500	PEV	C26-C25-C24	4.44	150.79	113.58
2	A	400	PEV	C26-C25-C24	4.44	150.77	113.58
2	B	500	PEV	O2-C31-C32	3.10	118.35	111.56
2	A	400	PEV	O2-C31-C32	3.09	118.32	111.56
2	B	500	PEV	C3-C2-C1	-2.87	105.32	111.86
2	A	400	PEV	C3-C2-C1	-2.87	105.33	111.86
2	B	500	PEV	O3-C11-C12	2.52	119.87	111.94
2	A	400	PEV	O3-C11-C12	2.51	119.83	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	POP	O2-P1-O	2.24	111.44	104.29
3	B	602	POP	O2-P1-O	2.14	111.09	104.29

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.

## 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, 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%)	0.57	22 (8%) 10 9	33, 57, 84, 95	0
1	B	250/277 (90%)	0.49	17 (6%) 17 17	25, 50, 71, 79	0
All	All	500/554 (90%)	0.53	39 (7%) 13 12	25, 53, 79, 95	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1595	GLY	10.0
1	A	1596	GLN	6.8
1	A	1604	TYR	5.3
1	A	1700	HIS	4.0
1	B	1771	CYS	3.9
1	A	1815	PRO	3.7
1	B	1597	ILE	3.7
1	A	1597	ILE	3.7
1	B	1770	ILE	3.3
1	B	1727	HIS	3.2
1	A	1594	THR	3.2
1	A	1727	HIS	3.1
1	B	1604	TYR	3.0
1	A	1579	LYS	3.0
1	B	1595	GLY	2.9
1	A	1696	GLU	2.9
1	A	1701	GLU	2.6
1	B	1620	ILE	2.5
1	B	1568	THR	2.5
1	B	1784	ASN	2.4
1	B	1683	LYS	2.4
1	A	1580	ALA	2.3
1	A	1692	GLY	2.3
1	A	1683	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1775	GLU	2.2
1	B	1696	GLU	2.2
1	B	1805	HIS	2.2
1	A	1794	GLN	2.2
1	B	1778	PHE	2.2
1	A	1601	LEU	2.2
1	A	1816	ASP	2.1
1	A	1814	GLN	2.1
1	B	1596	GLN	2.1
1	B	1690	CYS	2.1
1	B	1786	GLY	2.1
1	A	1568	THR	2.1
1	B	1779	THR	2.1
1	A	1726	ALA	2.0
1	A	1699	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PEV	B	500	49/49	0.38	4.06	20,71,84,86	3
2	PEV	A	400	49/49	0.34	3.84	20,71,84,86	3
3	POP	B	602	9/9	0.27	1.66	83,94,101,104	0
3	POP	B	601	9/9	0.19	-0.27	145,147,151,151	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.