



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:45 PM GMT

PDB ID : 1W2Z  
Title : PSAO and Xenon  
Authors : Duff, A.P.; Trambaiolo, D.M.; Cohen, A.E.; Ellis, P.J.; Juda, G.A.; Shepard, E.M.; Langley, D.B.; Dooley, D.M.; Freeman, H.C.; Guss, J.M.  
Deposited on : 2004-07-11  
Resolution : 2.24 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>

---

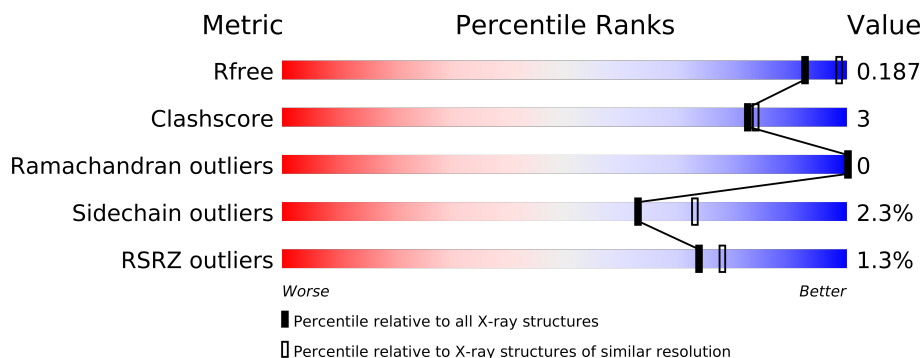
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.24 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	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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	649	
1	B	649	
1	C	649	
1	D	649	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	MN	A	702	-	X
4	XE	C	711	-	X
4	XE	D	711	-	X
5	NAG	A	1131	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	1558	-	X
5	NAG	B	1131	-	X
5	NAG	B	1558	-	X
5	NAG	D	1131	-	X
6	IOD	A	1649	-	X
6	IOD	A	1658	-	X
6	IOD	A	1661	-	X
6	IOD	A	1675	-	X
6	IOD	A	1678	-	X
6	IOD	A	1688	-	X
6	IOD	A	1690	-	X
6	IOD	B	1648	-	X
6	IOD	B	1660	-	X
6	IOD	B	1670	-	X
6	IOD	B	1672	-	X
6	IOD	B	1674	-	X
6	IOD	B	1676	-	X
6	IOD	B	1682	-	X
6	IOD	B	1688	-	X
6	IOD	B	1693	-	X
6	IOD	C	1654	-	X
6	IOD	C	1656	-	X
6	IOD	C	1657	-	X
6	IOD	C	1664	-	X
6	IOD	C	1665	-	X
6	IOD	C	1671	-	X
6	IOD	D	1650	-	X
6	IOD	D	1653	-	X
6	IOD	D	1665	-	X
6	IOD	D	1674	-	X
6	IOD	D	1688	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40764 atoms, of which 19073 are hydrogens 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 AMINE OXIDASE, COPPER CONTAINING.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	642	Total	C	H	N	O	S	9	7	0
			9956	3343	4750	879	972	12			
1	B	642	Total	C	H	N	O	S	4	8	0
			9948	3338	4748	879	971	12			
1	C	642	Total	C	H	N	O	S	4	7	0
			9942	3336	4746	879	969	12			
1	D	642	Total	C	H	N	O	S	6	8	0
			9941	3338	4741	879	971	12			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

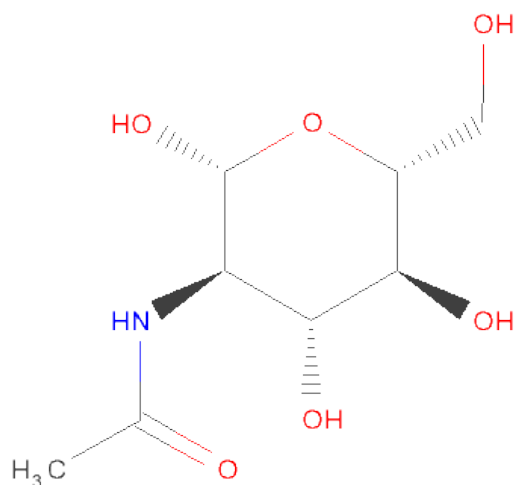
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Xe	0	0
			2	2		
4	A	2	Total	Xe	0	0
			2	2		
4	D	2	Total	Xe	0	0
			2	2		
4	C	2	Total	Xe	0	0
			2	2		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	A	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	B	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	B	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	C	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	C	1	Total	C	H	N	O	0	0
			25	8	11	1	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	D	1	Total	C	H	N	O	0	0
			25	8	11	1	5		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	48	Total	I	0	0
			48	48		
6	A	46	Total	I	0	0
			46	46		
6	D	42	Total	I	0	0
			42	42		
6	C	40	Total	I	0	0
			40	40		

- Molecule 7 is water.

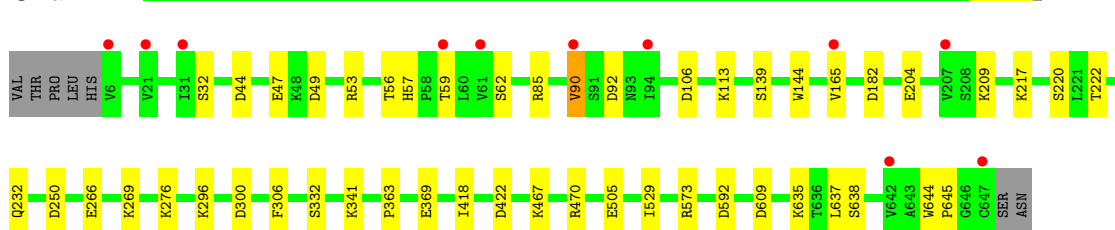
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	174	Total	O	0	0
			174	174		
7	B	141	Total	O	0	0
			141	141		
7	C	125	Total	O	0	0
			125	125		
7	D	145	Total	O	0	0
			145	145		

### 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.

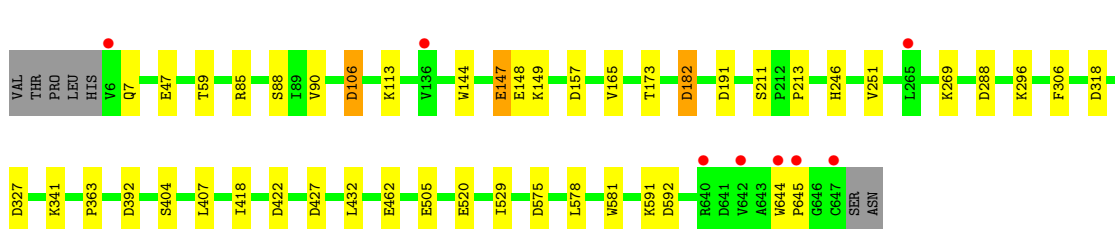
#### • Molecule 1: AMINE OXIDASE, COPPER CONTAINING

Chain A:



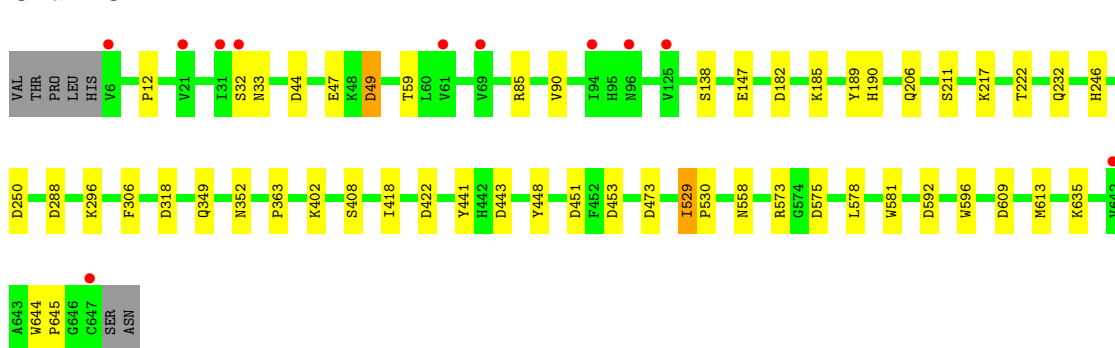
#### • Molecule 1: AMINE OXIDASE, COPPER CONTAINING

Chain B:



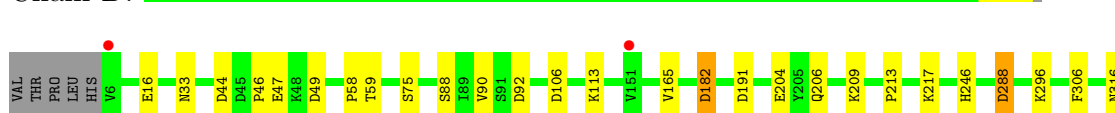
#### • Molecule 1: AMINE OXIDASE, COPPER CONTAINING

Chain C:



#### • Molecule 1: AMINE OXIDASE, COPPER CONTAINING

Chain D:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.51Å 196.27Å 89.67Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	29.88 – 2.24 29.82 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.88-2.24) 99.3 (29.82-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.224 0.172 , 0.187	Depositor DCC
$R_{free}$ test set	7082 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 9.2	EDS
Estimated twinning fraction	0.249 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 277759 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	40764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: NAG, MN, XE, TPQ, IOD, CU

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	0.58	0/5340	0.77	9/7270 (0.1%)
1	B	0.61	1/5347 (0.0%)	0.79	12/7280 (0.2%)
1	C	0.57	0/5339	0.78	13/7269 (0.2%)
1	D	0.58	0/5347	0.77	9/7280 (0.1%)
All	All	0.58	1/21373 (0.0%)	0.78	43/29099 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLU	CB-CG	-12.28	1.28	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	592	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	592	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	318	ASP	CB-CG-OD2	6.46	124.12	118.30
1	B	147	GLU	CA-CB-CG	6.46	127.60	113.40
1	C	49	ASP	CB-CG-OD2	6.42	124.08	118.30
1	D	288	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	250	ASP	CB-CG-OD2	6.39	124.06	118.30
1	B	288	ASP	CB-CG-OD2	6.37	124.03	118.30
1	D	106	ASP	CB-CG-OD2	6.25	123.93	118.30
1	C	288	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	592	ASP	CB-CG-OD2	6.24	123.92	118.30
1	D	609	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	250	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	106	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	575	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	609	ASP	CB-CG-OD2	5.77	123.49	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	453	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	106	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	44	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	443	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	451	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	182[A]	ASP	CB-CG-OD2	5.56	123.30	118.30
1	D	182[B]	ASP	CB-CG-OD2	5.56	123.30	118.30
1	D	592	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	609	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	318	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	92	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	427	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	157	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	575	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	191	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	147	GLU	CA-CB-CG	5.23	124.91	113.40
1	D	92	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	473	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	44	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	49	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	182	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	44	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	182[A]	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	182[B]	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	327	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	300	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	191	ASP	CB-CG-OD2	5.04	122.83	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	5206	4750	356	29	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5200	4748	359	31	0
1	C	5196	4746	358	32	0
1	D	5200	4741	366	29	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	28	22	6	0	0
5	B	28	22	6	0	0
5	C	28	22	6	0	0
5	D	28	22	6	0	0
6	A	46	0	0	26	0
6	B	48	0	0	29	0
6	C	40	0	0	19	0
6	D	42	0	0	26	0
7	A	174	0	0	2	0
7	B	141	0	0	6	0
7	C	125	0	0	3	0
7	D	145	0	0	3	0
All	All	21691	19073	1463	129	1

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 3.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:1692:IOD:I	6:B:1696:IOD:I	1.79	1.78
1:C:33:ASN:ND2	6:C:1686:IOD:I	2.27	1.37
1:D:182[A]:ASP:OD2	6:D:1676:IOD:I	2.20	1.30
1:C:613[B]:MET:CE	7:C:2065:HOH:O	1.72	1.28
1:C:182[B]:ASP:OD2	6:C:1668:IOD:I	2.24	1.26
1:B:182[A]:ASP:OD2	6:B:1675:IOD:I	2.26	1.23
6:D:1658:IOD:I	6:D:1684:IOD:I	3.04	1.15
1:C:422[A]:ASP:OD1	6:C:1673:IOD:I	2.37	1.13

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:422[A]:ASP:OD1	6:D:1672:IOD:I	2.38	1.12
1:C:613[B]:MET:HE1	7:C:2065:HOH:O	1.32	1.11
1:B:422[A]:ASP:OD1	6:B:1665:IOD:I	2.45	1.04
1:B:59[A]:THR:OG1	6:B:1666:IOD:I	2.46	1.03
1:A:422[A]:ASP:OD1	6:A:1676:IOD:I	2.47	1.02
1:D:463:LYS:NZ	6:D:1680:IOD:I	2.63	1.01
1:D:59[B]:THR:OG1	6:D:1662:IOD:I	2.50	0.97
6:A:1655:IOD:I	7:A:2021:HOH:O	2.54	0.96
1:C:59[B]:THR:OG1	6:C:1669:IOD:I	2.52	0.95
1:A:113:LYS:HG2	6:A:1687:IOD:I	2.37	0.95
1:C:182[B]:ASP:CG	6:C:1668:IOD:I	2.79	0.90
1:D:113:LYS:HG2	6:D:1686:IOD:I	2.43	0.88
6:A:1688:IOD:I	7:A:2132:HOH:O	2.64	0.84
6:B:1675:IOD:I	7:B:2015:HOH:O	2.65	0.84
1:B:113:LYS:HG2	6:B:1686:IOD:I	2.51	0.80
1:C:613[B]:MET:HE3	7:C:2065:HOH:O	1.49	0.75
1:C:222:THR:HG22	6:D:1652:IOD:I	2.57	0.74
1:A:59[A]:THR:OG1	6:A:1683:IOD:I	2.75	0.71
1:C:182[B]:ASP:OD1	6:C:1668:IOD:I	2.80	0.70
1:D:182[A]:ASP:CG	6:D:1676:IOD:I	3.00	0.69
6:B:1673:IOD:I	7:B:2047:HOH:O	2.82	0.67
1:C:85:ARG:HD3	6:C:1680:IOD:I	2.64	0.67
1:C:363:PRO:HG2	6:D:1686:IOD:I	2.66	0.66
1:B:182[A]:ASP:CG	6:B:1675:IOD:I	3.04	0.65
1:B:165:VAL:HG21	6:B:1694:IOD:I	2.67	0.65
1:C:59[A]:THR:HB	6:C:1669:IOD:I	2.66	0.65
1:B:7:GLN:HG2	6:B:1690:IOD:I	2.68	0.64
1:A:505:GLU:HG2	6:A:1692:IOD:I	2.70	0.62
1:C:33:ASN:CG	6:C:1686:IOD:I	3.08	0.62
1:C:418:ILE:HD12	6:C:1663:IOD:I	2.69	0.62
1:D:629:GLU:OE1	7:D:2142:HOH:O	2.16	0.60
1:A:363:PRO:HG2	6:B:1686:IOD:I	2.72	0.59
1:A:635:LYS:NZ	6:B:1684:IOD:I	3.02	0.59
1:A:638:SER:N	6:A:1674:IOD:I	3.00	0.59
1:B:59[B]:THR:HB	6:B:1666:IOD:I	2.72	0.59
6:A:1687:IOD:I	1:B:363:PRO:HG2	2.73	0.58
1:B:213:PRO:HA	6:B:1663:IOD:I	2.73	0.58
1:A:418:ILE:CD1	6:A:1667:IOD:I	3.21	0.58
1:B:147:GLU:CB	6:B:1678:IOD:I	3.22	0.57
1:B:173:THR:HG23	6:B:1685:IOD:I	2.74	0.57
1:A:418:ILE:HD13	6:A:1667:IOD:I	2.74	0.57
1:A:57:HIS:HA	6:A:1683:IOD:I	2.74	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:1666:IOD:I	7:D:2049:HOH:O	2.87	0.56
1:A:85:ARG:HD3	6:A:1679:IOD:I	2.76	0.56
1:C:222:THR:CG2	6:D:1652:IOD:I	3.23	0.56
1:D:206:GLN:NE2	6:D:1689:IOD:I	2.94	0.56
1:C:418:ILE:CD1	6:C:1663:IOD:I	3.24	0.55
1:A:62:SER:OG	1:A:85:ARG:NH2	2.40	0.55
1:B:211:SER:N	6:B:1684:IOD:I	3.01	0.55
1:D:418:ILE:CD1	6:D:1659:IOD:I	3.25	0.54
1:D:59[A]:THR:HB	6:D:1662:IOD:I	2.77	0.54
1:A:369:GLU:HA	6:A:1684:IOD:I	2.78	0.54
1:D:213:PRO:HA	6:D:1657:IOD:I	2.78	0.54
1:A:332:SER:HB2	6:A:1690:IOD:I	2.78	0.53
1:B:113:LYS:CG	6:B:1686:IOD:I	3.24	0.53
1:A:222:THR:HG22	6:B:1652:IOD:I	2.79	0.53
1:C:59[B]:THR:HG22	6:C:1669:IOD:I	2.79	0.53
1:B:165:VAL:CG2	6:B:1694:IOD:I	3.27	0.52
1:D:418:ILE:HD13	6:D:1659:IOD:I	2.80	0.52
6:B:1668:IOD:I	6:B:1692:IOD:I	3.67	0.52
1:A:165:VAL:HG21	6:A:1691:IOD:I	2.81	0.51
1:C:206:GLN:NE2	6:C:1687:IOD:I	3.01	0.51
1:B:432:LEU:N	6:B:1691:IOD:I	3.04	0.51
1:B:106:ASP:OD1	7:B:2019:HOH:O	2.19	0.51
1:D:75:SER:OG	6:D:1675:IOD:I	2.96	0.49
1:A:418:ILE:HD12	6:A:1667:IOD:I	2.83	0.49
1:C:529:ILE:HG13	1:C:530:PRO:HD2	1.95	0.49
1:A:53:ARG:HG3	6:A:1685:IOD:I	2.83	0.49
1:B:392:ASP:HB2	1:B:404:SER:OG	2.13	0.48
1:B:147:GLU:HB3	6:B:1678:IOD:I	2.84	0.48
1:D:49:ASP:HB3	6:D:1673:IOD:I	2.84	0.48
1:A:90:VAL:HG13	6:A:1653:IOD:I	2.84	0.47
1:C:352:ASN:HA	6:C:1682:IOD:I	2.85	0.47
1:B:246:HIS:HB2	6:B:1656:IOD:I	2.84	0.47
1:D:463:LYS:CE	6:D:1680:IOD:I	3.33	0.46
1:C:90:VAL:HG13	6:C:1651:IOD:I	2.86	0.46
1:A:217:LYS:HD3	6:A:1677:IOD:I	2.86	0.46
1:A:644:TRP:CD2	1:A:645:PRO:HA	2.50	0.45
1:D:204:GLU:HG2	1:D:209:LYS:CB	2.47	0.45
1:B:85:ARG:HD3	6:B:1687:IOD:I	2.87	0.45
1:C:644:TRP:CD2	1:C:645:PRO:HA	2.52	0.45
1:D:58:PRO:HD2	6:D:1662:IOD:I	2.87	0.45
1:D:165:VAL:HG21	6:D:1689:IOD:I	2.87	0.44
1:B:182[A]:ASP:OD2	7:B:2036:HOH:O	2.20	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:246:HIS:HB2	6:C:1676:IOD:I	2.87	0.44
1:D:217:LYS:HD3	6:D:1671:IOD:I	2.88	0.44
1:B:462:GLU:OE2	1:B:520:GLU:OE1	2.35	0.44
1:A:113:LYS:CG	6:A:1687:IOD:I	3.25	0.44
1:A:637:LEU:HA	6:A:1674:IOD:I	2.88	0.44
1:B:578:LEU:HA	1:B:581:TRP:CE3	2.53	0.43
1:B:85:ARG:HB2	6:B:1687:IOD:I	2.88	0.43
1:A:276:LYS:NZ	6:A:1686:IOD:I	3.19	0.43
1:A:59[B]:THR:HB	6:A:1683:IOD:I	2.88	0.43
1:C:402:LYS:HD3	6:C:1666:IOD:I	2.88	0.43
1:D:316:ASN:ND2	1:D:321:PRO:HA	2.34	0.43
1:D:418:ILE:HD12	6:D:1659:IOD:I	2.89	0.43
1:D:46:PRO:HG3	7:D:2004:HOH:O	2.20	0.42
1:B:251:VAL:HG12	7:B:2011:HOH:O	2.20	0.42
1:D:316:ASN:HD22	1:D:321:PRO:HA	1.84	0.42
1:D:246:HIS:HB2	6:D:1665:IOD:I	2.89	0.42
1:D:458:HIS:HB3	1:D:590:ASN:OD1	2.19	0.42
1:B:644:TRP:CD1	1:B:645:PRO:HD2	2.55	0.42
1:D:288:ASP:OD1	1:D:288:ASP:C	2.58	0.42
1:D:165:VAL:CG2	6:D:1689:IOD:I	3.38	0.41
1:A:165:VAL:CG2	6:A:1691:IOD:I	3.39	0.41
1:D:204:GLU:HG2	1:D:209:LYS:HB3	2.01	0.41
6:D:1670:IOD:I	6:D:1687:IOD:I	3.78	0.41
1:C:189:TYR:O	1:C:190[B]:HIS:CD2	2.74	0.41
1:B:505:GLU:HG2	6:B:1682:IOD:I	2.91	0.41
1:C:448:TYR:O	1:C:596:TRP:HA	2.21	0.41
1:B:148:GLU:O	7:B:2025:HOH:O	2.22	0.41
1:B:418:ILE:HD13	6:B:1662:IOD:I	2.91	0.41
1:A:204:GLU:CG	1:A:209:LYS:HB2	2.51	0.41
1:A:217:LYS:CD	6:A:1677:IOD:I	3.39	0.40
1:C:441:TYR:HB3	1:D:482:TRP:CH2	2.56	0.40
1:C:418:ILE:HD13	6:C:1663:IOD:I	2.92	0.40
1:B:144:TRP:CD1	6:B:1678:IOD:I	3.44	0.40
1:C:558:ASN:HA	6:C:1677:IOD:I	2.90	0.40
1:C:578:LEU:HA	1:C:581:TRP:CE3	2.57	0.40
1:A:144:TRP:CD1	1:A:573:ARG:CZ	3.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:470:ARG:O	1:D:537:GLU:OE1[2_646]	2.18	0.02

## 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	645/649 (99%)	629 (98%)	16 (2%)	0	100	100
1	B	646/649 (100%)	628 (97%)	18 (3%)	0	100	100
1	C	645/649 (99%)	630 (98%)	15 (2%)	0	100	100
1	D	646/649 (100%)	627 (97%)	19 (3%)	0	100	100
All	All	2582/2596 (100%)	2514 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	581/582 (100%)	567 (98%)	14 (2%)	61	72
1	B	582/582 (100%)	571 (98%)	11 (2%)	69	79
1	C	581/582 (100%)	566 (97%)	15 (3%)	59	70
1	D	582/582 (100%)	569 (98%)	13 (2%)	64	75
All	All	2326/2328 (100%)	2273 (98%)	53 (2%)	63	73

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	47	GLU
1	A	56	THR
1	A	90	VAL
1	A	139	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	220	SER
1	A	232	GLN
1	A	266	GLU
1	A	269	LYS
1	A	296	LYS
1	A	306	PHE
1	A	341	LYS
1	A	467	LYS
1	A	529	ILE
1	B	47	GLU
1	B	88	SER
1	B	90	VAL
1	B	149	LYS
1	B	269	LYS
1	B	296	LYS
1	B	306	PHE
1	B	341	LYS
1	B	407	LEU
1	B	529	ILE
1	B	591	LYS
1	C	12	PRO
1	C	32	SER
1	C	47	GLU
1	C	49	ASP
1	C	138	SER
1	C	185	LYS
1	C	211	SER
1	C	217	LYS
1	C	232	GLN
1	C	296	LYS
1	C	306	PHE
1	C	349	GLN
1	C	529	ILE
1	C	573	ARG
1	C	635	LYS
1	D	16	GLU
1	D	33	ASN
1	D	47	GLU
1	D	88	SER
1	D	90	VAL
1	D	296	LYS
1	D	306	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	341	LYS
1	D	472	LYS
1	D	559	ARG
1	D	619	SER
1	D	635	LYS
1	D	641	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	364	ASN
1	A	519	ASN
1	B	316	ASN
1	C	316	ASN
1	D	227	GLN
1	D	316	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

9 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPQ	A	387[A]	-	7,9,15	2.58	5 (71%)	8,12,21	1.46	2 (25%)
1	TPQ	A	387[B]	-	7,9,15	2.46	5 (71%)	8,12,21	1.03	0
1	TPQ	A	387[C]	-	7,9,15	2.58	5 (71%)	8,12,21	1.46	2 (25%)
1	TPQ	B	387[A]	-	7,9,15	2.67	4 (57%)	8,12,21	1.32	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPQ	B	387[B]	-	7,9,15	2.55	4 (57%)	8,12,21	1.01	1 (12%)
1	TPQ	C	387[A]	-	7,9,15	2.88	5 (71%)	8,12,21	0.86	0
1	TPQ	C	387[B]	-	7,9,15	2.44	4 (57%)	8,12,21	1.07	0
1	TPQ	D	387[A]	-	7,9,15	2.71	5 (71%)	8,12,21	1.10	0
1	TPQ	D	387[B]	-	7,9,15	2.57	5 (71%)	8,12,21	1.22	1 (12%)

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
1	TPQ	A	387[A]	-	-	0/0/13/24	0/1/1/1
1	TPQ	A	387[B]	-	-	0/0/13/24	0/1/1/1
1	TPQ	A	387[C]	-	-	0/0/13/24	0/1/1/1
1	TPQ	B	387[A]	-	-	0/0/13/24	0/1/1/1
1	TPQ	B	387[B]	-	-	0/0/13/24	0/1/1/1
1	TPQ	C	387[A]	-	-	0/0/13/24	0/1/1/1
1	TPQ	C	387[B]	-	-	0/0/13/24	0/1/1/1
1	TPQ	D	387[A]	-	-	0/0/13/24	0/1/1/1
1	TPQ	D	387[B]	-	-	0/0/13/24	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	387[A]	TPQ	C6-C5	4.34	1.51	1.42
1	B	387[A]	TPQ	C6-C5	4.27	1.51	1.42
1	D	387[A]	TPQ	C6-C5	3.98	1.50	1.42
1	A	387[C]	TPQ	C6-C5	3.78	1.50	1.42
1	A	387[A]	TPQ	C6-C5	3.76	1.50	1.42
1	B	387[B]	TPQ	C6-C5	3.69	1.49	1.42
1	A	387[B]	TPQ	O4-C4	-3.49	1.25	1.34
1	B	387[B]	TPQ	O4-C4	-3.48	1.25	1.34
1	C	387[B]	TPQ	O4-C4	-3.45	1.25	1.34
1	A	387[C]	TPQ	C3-C2	3.44	1.49	1.42
1	C	387[A]	TPQ	C3-C2	3.44	1.49	1.42
1	D	387[B]	TPQ	C3-C2	3.41	1.49	1.42
1	A	387[A]	TPQ	C3-C2	3.40	1.49	1.42
1	D	387[A]	TPQ	C3-C2	3.32	1.49	1.42
1	D	387[B]	TPQ	O4-C4	-3.32	1.25	1.34
1	B	387[A]	TPQ	O4-C4	-3.28	1.25	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387[A]	TPQ	C3-C2	3.26	1.49	1.42
1	A	387[B]	TPQ	C6-C5	3.26	1.49	1.42
1	C	387[B]	TPQ	C6-C5	3.25	1.49	1.42
1	C	387[A]	TPQ	O4-C4	-3.19	1.25	1.34
1	D	387[B]	TPQ	C6-C5	3.09	1.48	1.42
1	D	387[A]	TPQ	O4-C4	-3.07	1.26	1.34
1	C	387[B]	TPQ	C3-C2	3.03	1.48	1.42
1	B	387[B]	TPQ	C3-C2	3.02	1.48	1.42
1	A	387[B]	TPQ	C3-C2	2.93	1.48	1.42
1	D	387[B]	TPQ	C3-C4	2.91	1.40	1.35
1	C	387[A]	TPQ	O2-C2	2.89	1.26	1.22
1	A	387[A]	TPQ	C3-C4	2.84	1.40	1.35
1	A	387[C]	TPQ	C3-C4	2.82	1.40	1.35
1	A	387[A]	TPQ	O4-C4	-2.76	1.26	1.34
1	A	387[C]	TPQ	O4-C4	-2.74	1.27	1.34
1	C	387[A]	TPQ	C3-C4	2.73	1.40	1.35
1	D	387[A]	TPQ	C3-C4	2.72	1.40	1.35
1	B	387[B]	TPQ	C3-C4	2.69	1.40	1.35
1	D	387[A]	TPQ	O2-C2	2.67	1.26	1.22
1	B	387[A]	TPQ	C3-C4	2.60	1.39	1.35
1	C	387[B]	TPQ	C3-C4	2.60	1.39	1.35
1	A	387[B]	TPQ	C3-C4	2.36	1.39	1.35
1	D	387[B]	TPQ	O2-C2	2.22	1.25	1.22
1	A	387[B]	TPQ	O2-C2	2.20	1.25	1.22
1	A	387[A]	TPQ	O2-C2	2.18	1.25	1.22
1	A	387[C]	TPQ	O2-C2	2.12	1.25	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387[A]	TPQ	C3-C4-C5	-2.39	118.64	121.27
1	A	387[C]	TPQ	C3-C4-C5	-2.37	118.66	121.27
1	B	387[A]	TPQ	C4-C3-C2	-2.35	119.36	121.61
1	A	387[A]	TPQ	C6-C5-C4	2.16	121.02	117.44
1	A	387[C]	TPQ	C6-C5-C4	2.16	121.00	117.44
1	B	387[B]	TPQ	C4-C3-C2	-2.13	119.57	121.61
1	D	387[B]	TPQ	C4-C3-C2	-2.05	119.64	121.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 200 ligands modelled in this entry, 192 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	1131	1	12,14,15	0.58	0	15,19,21	1.05	0
5	NAG	A	1558	1	12,14,15	0.52	0	15,19,21	1.37	3 (20%)
5	NAG	B	1131	1	12,14,15	0.63	0	15,19,21	0.96	0
5	NAG	B	1558	1	12,14,15	0.47	0	15,19,21	1.16	2 (13%)
5	NAG	C	1131	1	12,14,15	0.60	0	15,19,21	1.07	0
5	NAG	C	1558	1	12,14,15	0.55	0	15,19,21	1.09	1 (6%)
5	NAG	D	1131	1	12,14,15	0.55	0	15,19,21	1.02	0
5	NAG	D	1558	1	12,14,15	0.71	1 (8%)	15,19,21	1.48	3 (20%)

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
5	NAG	A	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1558	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1558	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1558	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1558	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1558	NAG	O5-C5	-2.05	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1558	NAG	O5-C5-C6	3.65	110.81	106.98
5	A	1558	NAG	O5-C5-C6	3.24	110.39	106.98
5	D	1558	NAG	O5-C5-C4	-3.10	106.72	110.65
5	C	1558	NAG	O5-C5-C6	3.00	110.13	106.98
5	D	1558	NAG	C3-C2-N2	-2.46	108.01	111.76
5	A	1558	NAG	O5-C5-C4	2.41	113.71	110.65
5	B	1558	NAG	O5-C5-C4	2.29	113.56	110.65
5	A	1558	NAG	C3-C4-C5	2.25	114.21	110.20
5	B	1558	NAG	O5-C5-C6	2.13	109.22	106.98

There are no chirality outliers.

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	642/649 (98%)	-0.07	11 (1%) 67 71	10, 18, 31, 50	2 (0%)
1	B	642/649 (98%)	-0.05	8 (1%) 75 80	9, 18, 32, 50	2 (0%)
1	C	642/649 (98%)	-0.01	11 (1%) 67 71	10, 18, 32, 50	2 (0%)
1	D	642/649 (98%)	-0.03	5 (0%) 83 86	9, 18, 32, 50	2 (0%)
All	All	2568/2596 (98%)	-0.04	35 (1%) 74 76	9, 18, 32, 50	8 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	VAL	4.5
1	A	647	CYS	3.9
1	D	647	CYS	3.8
1	B	647	CYS	3.7
1	B	642	VAL	3.4
1	D	6	VAL	3.3
1	C	61	VAL	2.8
1	A	642	VAL	2.7
1	B	644	TRP	2.7
1	A	31	ILE	2.7
1	C	647	CYS	2.5
1	A	6	VAL	2.5
1	D	151	VAL	2.5
1	B	136	VAL	2.5
1	D	642	VAL	2.5
1	C	32	SER	2.4
1	D	366	SER	2.4
1	C	31	ILE	2.3
1	A	61	VAL	2.3
1	C	125	VAL	2.3
1	A	59[A]	THR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	6	VAL	2.3
1	C	94	ILE	2.2
1	A	90	VAL	2.2
1	B	640	ARG	2.2
1	C	96	ASN	2.2
1	B	265	LEU	2.1
1	C	69	VAL	2.1
1	A	21	VAL	2.1
1	A	165	VAL	2.1
1	C	21	VAL	2.1
1	A	207	VAL	2.0
1	C	642	VAL	2.0
1	A	94	ILE	2.0
1	B	645	PRO	2.0

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

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
1	TPQ	A	387[A]	9/15	0.18	2.26	26,29,30,35	11
1	TPQ	C	387[A]	9/15	0.20	2.22	25,28,32,35	11
1	TPQ	C	387[B]	9/15	0.20	2.22	23,27,30,32	11
1	TPQ	A	387[B]	9/15	0.18	1.56	24,27,30,32	11
1	TPQ	A	387[C]	9/15	0.18	1.40	0,0,0,0	9
1	TPQ	D	387[B]	9/15	0.18	1.15	24,27,30,32	11
1	TPQ	D	387[A]	9/15	0.18	1.15	26,29,32,35	11
1	TPQ	B	387[B]	9/15	0.18	1.07	24,27,30,32	11
1	TPQ	B	387[A]	9/15	0.18	0.88	26,29,31,35	11

## 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
6	IOD	D	1688	1/1	0.20	14.10	38,38,38,38	1
6	IOD	C	1657	1/1	0.18	11.62	90,90,90,90	1
6	IOD	A	1675	1/1	0.21	9.45	87,87,87,87	1
6	IOD	B	1674	1/1	0.18	7.76	48,48,48,48	1
6	IOD	B	1648	1/1	0.17	7.33	36,36,36,36	0
6	IOD	D	1674	1/1	0.21	7.02	40,40,40,40	1
6	IOD	B	1676	1/1	0.17	6.29	47,47,47,47	1
5	NAG	B	1131	14/15	0.19	6.14	60,66,77,78	0
6	IOD	B	1688	1/1	0.17	5.97	42,42,42,42	1
6	IOD	D	1650	1/1	0.19	5.51	37,37,37,37	0
6	IOD	A	1649	1/1	0.18	5.37	47,47,47,47	0
6	IOD	C	1654	1/1	0.15	4.98	51,51,51,51	1
6	IOD	A	1690	1/1	0.17	4.08	55,55,55,55	1
6	IOD	B	1672	1/1	0.20	3.74	40,40,40,40	1
4	XE	C	711	1/1	0.27	3.46	49,49,49,49	1
5	NAG	B	1558	14/15	0.22	3.27	59,71,80,80	0
4	XE	D	711	1/1	0.28	3.24	55,55,55,55	1
6	IOD	B	1670	1/1	0.20	2.91	42,42,42,42	1
6	IOD	A	1688	1/1	0.20	2.72	47,47,47,47	1
6	IOD	D	1653	1/1	0.18	2.71	45,45,45,45	1
5	NAG	D	1131	14/15	0.20	2.59	58,66,76,77	0
6	IOD	A	1658	1/1	0.17	2.56	44,44,44,44	1
6	IOD	C	1656	1/1	0.19	2.52	48,48,48,48	1
6	IOD	B	1682	1/1	0.20	2.52	72,72,72,72	1
6	IOD	C	1665	1/1	0.19	2.52	49,49,49,49	1
6	IOD	C	1671	1/1	0.16	2.51	67,67,67,67	1
6	IOD	A	1661	1/1	0.18	2.37	51,51,51,51	1
6	IOD	C	1664	1/1	0.17	2.35	43,43,43,43	1
6	IOD	A	1678	1/1	0.16	2.29	43,43,43,43	1
5	NAG	A	1558	14/15	0.26	2.28	62,78,83,83	0
3	MN	A	702	1/1	0.18	2.27	36,36,36,36	0
6	IOD	B	1693	1/1	0.19	2.26	42,42,42,42	1
6	IOD	B	1660	1/1	0.17	2.20	40,40,40,40	1
5	NAG	A	1131	14/15	0.18	2.14	48,58,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	IOD	D	1665	1/1	0.18	2.03	45,45,45,45	1
5	NAG	D	1558	14/15	0.22	1.92	71,84,87,88	0
6	IOD	A	1669	1/1	0.15	1.90	71,71,71,71	1
5	NAG	C	1131	14/15	0.18	1.84	54,64,70,79	0
4	XE	A	710	1/1	0.18	1.82	32,32,32,32	1
6	IOD	B	1653	1/1	0.14	1.80	55,55,55,55	1
6	IOD	B	1661	1/1	0.15	1.79	47,47,47,47	1
6	IOD	D	1677	1/1	0.26	1.78	53,53,53,53	1
6	IOD	D	1684	1/1	0.19	1.72	44,44,44,44	1
5	NAG	C	1558	14/15	0.22	1.67	69,83,88,88	0
6	IOD	C	1670	1/1	0.18	1.67	55,55,55,55	1
4	XE	D	710	1/1	0.18	1.66	33,33,33,33	1
6	IOD	D	1655	1/1	0.15	1.48	50,50,50,50	1
6	IOD	D	1681	1/1	0.15	1.46	64,64,64,64	1
6	IOD	C	1676	1/1	0.22	1.46	57,57,57,57	1
6	IOD	A	1648	1/1	0.18	1.45	39,39,39,39	0
6	IOD	B	1687	1/1	0.22	1.40	51,51,51,51	1
6	IOD	C	1668	1/1	0.17	1.39	41,41,41,41	1
6	IOD	B	1679	1/1	0.18	1.37	37,37,37,37	1
6	IOD	B	1690	1/1	0.21	1.34	65,65,65,65	1
6	IOD	C	1659	1/1	0.16	1.34	51,51,51,51	1
6	IOD	B	1685	1/1	0.13	1.32	66,66,66,66	1
4	XE	B	710	1/1	0.17	1.31	35,35,35,35	1
6	IOD	D	1657	1/1	0.19	1.31	39,39,39,39	1
6	IOD	B	1669	1/1	0.16	1.29	66,66,66,66	1
6	IOD	B	1691	1/1	0.15	1.27	50,50,50,50	1
6	IOD	D	1661	1/1	0.14	1.25	48,48,48,48	1
6	IOD	C	1682	1/1	0.20	1.24	41,41,41,41	1
2	CU	C	701	1/1	0.18	1.24	33,33,33,33	0
6	IOD	B	1681	1/1	0.17	1.23	40,40,40,40	1
6	IOD	A	1662	1/1	0.19	1.21	46,46,46,46	1
6	IOD	B	1651	1/1	0.16	1.19	47,47,47,47	1
2	CU	A	701	1/1	0.18	1.18	34,34,34,34	0
6	IOD	A	1650	1/1	0.20	1.13	45,45,45,45	0
6	IOD	A	1657	1/1	0.14	1.12	48,48,48,48	1
6	IOD	A	1687	1/1	0.20	1.11	78,78,78,78	1
6	IOD	D	1664	1/1	0.17	1.09	50,50,50,50	1
3	MN	C	702	1/1	0.14	0.98	35,35,35,35	0
6	IOD	D	1671	1/1	0.16	0.97	37,37,37,37	1
6	IOD	B	1689	1/1	0.16	0.97	34,34,34,34	1
6	IOD	B	1673	1/1	0.20	0.96	56,56,56,56	1
6	IOD	C	1652	1/1	0.19	0.88	44,44,44,44	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	A	1695	1/1	0.17	0.88	48,48,48,48	1
6	IOD	B	1678	1/1	0.17	0.86	59,59,59,59	1
6	IOD	A	1659	1/1	0.15	0.86	51,51,51,51	1
6	IOD	C	1685	1/1	0.14	0.86	40,40,40,40	1
6	IOD	D	1663	1/1	0.16	0.85	64,64,64,64	1
6	IOD	A	1653	1/1	0.21	0.85	78,78,78,78	1
6	IOD	D	1658	1/1	0.16	0.85	50,50,50,50	1
6	IOD	C	1648	1/1	0.16	0.83	47,47,47,47	0
4	XE	C	710	1/1	0.17	0.82	32,32,32,32	1
2	CU	B	701	1/1	0.17	0.81	31,31,31,31	0
6	IOD	B	1671	1/1	0.17	0.79	49,49,49,49	1
6	IOD	A	1652	1/1	0.19	0.78	39,39,39,39	0
6	IOD	B	1692	1/1	0.21	0.76	59,59,59,59	1
6	IOD	C	1649	1/1	0.15	0.73	42,42,42,42	0
6	IOD	C	1650	1/1	0.18	0.72	37,37,37,37	0
6	IOD	A	1672	1/1	0.14	0.71	77,77,77,77	1
6	IOD	B	1649	1/1	0.19	0.67	43,43,43,43	0
6	IOD	B	1656	1/1	0.15	0.65	49,49,49,49	1
3	MN	D	702	1/1	0.14	0.62	36,36,36,36	0
6	IOD	D	1659	1/1	0.17	0.58	92,92,92,92	1
6	IOD	D	1670	1/1	0.18	0.58	47,47,47,47	1
6	IOD	A	1689	1/1	0.19	0.58	50,50,50,50	1
2	CU	D	701	1/1	0.16	0.54	29,29,29,29	0
6	IOD	A	1667	1/1	0.16	0.53	78,78,78,78	1
6	IOD	C	1686	1/1	0.14	0.52	42,42,42,42	1
4	XE	A	711	1/1	0.17	0.51	47,47,47,47	1
6	IOD	C	1655	1/1	0.13	0.51	130,130,130,130	1
4	XE	B	711	1/1	0.17	0.49	51,51,51,51	1
6	IOD	D	1660	1/1	0.15	0.41	74,74,74,74	1
6	IOD	A	1674	1/1	0.14	0.40	53,53,53,53	1
6	IOD	D	1656	1/1	0.14	0.39	44,44,44,44	1
6	IOD	B	1683	1/1	0.13	0.39	70,70,70,70	1
6	IOD	A	1681	1/1	0.16	0.34	50,50,50,50	1
6	IOD	D	1648	1/1	0.16	0.34	52,52,52,52	0
6	IOD	A	1680	1/1	0.15	0.34	60,60,60,60	1
6	IOD	D	1654	1/1	0.17	0.33	52,52,52,52	1
6	IOD	B	1659	1/1	0.13	0.33	54,54,54,54	1
6	IOD	A	1651	1/1	0.17	0.32	52,52,52,52	0
6	IOD	A	1686	1/1	0.13	0.30	43,43,43,43	1
6	IOD	C	1662	1/1	0.13	0.25	49,49,49,49	1
6	IOD	C	1667	1/1	0.18	0.24	61,61,61,61	1
6	IOD	D	1678	1/1	0.18	0.22	40,40,40,40	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	D	1672	1/1	0.17	0.20	51,51,51,51	1
6	IOD	C	1674	1/1	0.14	0.16	57,57,57,57	1
6	IOD	B	1677	1/1	0.19	0.16	54,54,54,54	1
6	IOD	A	1677	1/1	0.15	0.15	47,47,47,47	1
6	IOD	D	1669	1/1	0.16	0.14	68,68,68,68	1
6	IOD	A	1660	1/1	0.18	0.13	121,121,121,121	1
6	IOD	B	1663	1/1	0.13	0.10	44,44,44,44	1
6	IOD	B	1665	1/1	0.13	0.07	46,46,46,46	1
6	IOD	B	1657	1/1	0.13	0.03	74,74,74,74	1
6	IOD	A	1665	1/1	0.15	0.02	53,53,53,53	1
6	IOD	C	1680	1/1	0.16	0.01	50,50,50,50	1
6	IOD	C	1683	1/1	0.15	-0.00	55,55,55,55	1
6	IOD	B	1654	1/1	0.15	-0.03	48,48,48,48	1
6	IOD	C	1684	1/1	0.13	-0.05	49,49,49,49	1
6	IOD	C	1653	1/1	0.15	-0.07	45,45,45,45	1
6	IOD	A	1664	1/1	0.11	-0.08	55,55,55,55	1
6	IOD	B	1680	1/1	0.12	-0.10	41,41,41,41	1
3	MN	B	702	1/1	0.12	-0.11	33,33,33,33	0
6	IOD	C	1679	1/1	0.16	-0.13	67,67,67,67	1
6	IOD	A	1655	1/1	0.15	-0.13	47,47,47,47	1
6	IOD	B	1662	1/1	0.16	-0.21	68,68,68,68	1
6	IOD	C	1681	1/1	0.12	-0.24	49,49,49,49	1
6	IOD	B	1650	1/1	0.13	-0.30	82,82,82,82	1
6	IOD	A	1679	1/1	0.14	-0.31	53,53,53,53	1
6	IOD	C	1651	1/1	0.15	-0.32	82,82,82,82	0
6	IOD	C	1661	1/1	0.13	-0.34	48,48,48,48	1
6	IOD	D	1662	1/1	0.15	-0.35	56,56,56,56	1
6	IOD	D	1683	1/1	0.14	-0.36	50,50,50,50	1
6	IOD	A	1663	1/1	0.13	-0.37	62,62,62,62	1
6	IOD	D	1651	1/1	0.15	-0.39	72,72,72,72	1
6	IOD	B	1655	1/1	0.14	-0.40	75,75,75,75	1
6	IOD	D	1667	1/1	0.12	-0.41	58,58,58,58	1
6	IOD	D	1652	1/1	0.16	-0.43	53,53,53,53	1
6	IOD	A	1684	1/1	0.12	-0.45	67,67,67,67	1
6	IOD	D	1666	1/1	0.14	-0.49	61,61,61,61	1
6	IOD	C	1666	1/1	0.11	-0.49	54,54,54,54	1
6	IOD	D	1676	1/1	0.14	-0.50	39,39,39,39	1
6	IOD	A	1670	1/1	0.10	-0.51	63,63,63,63	1
6	IOD	B	1658	1/1	0.11	-0.52	77,77,77,77	1
6	IOD	A	1671	1/1	0.10	-0.53	71,71,71,71	1
6	IOD	D	1668	1/1	0.18	-0.55	76,76,76,76	1
6	IOD	B	1664	1/1	0.15	-0.58	61,61,61,61	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	D	1679	1/1	0.11	-0.58	49,49,49,49	1
6	IOD	A	1676	1/1	0.15	-0.59	55,55,55,55	1
6	IOD	A	1666	1/1	0.12	-0.60	49,49,49,49	1
6	IOD	B	1666	1/1	0.14	-0.60	47,47,47,47	1
6	IOD	B	1675	1/1	0.14	-0.61	43,43,43,43	1
6	IOD	B	1668	1/1	0.13	-0.61	48,48,48,48	1
6	IOD	D	1649	1/1	0.13	-0.62	52,52,52,52	0
6	IOD	A	1654	1/1	0.14	-0.63	83,83,83,83	1
6	IOD	B	1686	1/1	0.13	-0.66	50,50,50,50	1
6	IOD	A	1656	1/1	0.13	-0.69	45,45,45,45	1
6	IOD	C	1658	1/1	0.12	-0.71	68,68,68,68	1
6	IOD	D	1682	1/1	0.11	-0.74	47,47,47,47	1
6	IOD	B	1667	1/1	0.15	-0.74	82,82,82,82	1
6	IOD	C	1672	1/1	0.10	-0.80	50,50,50,50	1
6	IOD	C	1669	1/1	0.12	-0.83	74,74,74,74	1
6	IOD	C	1663	1/1	0.12	-0.94	57,57,57,57	1
6	IOD	C	1660	1/1	0.09	-0.96	103,103,103,103	1
6	IOD	A	1673	1/1	0.12	-0.97	62,62,62,62	1
6	IOD	B	1652	1/1	0.12	-1.02	57,57,57,57	1
6	IOD	A	1683	1/1	0.11	-1.07	61,61,61,61	1
6	IOD	D	1685	1/1	0.11	-1.11	40,40,40,40	1
6	IOD	D	1680	1/1	0.10	-1.12	51,51,51,51	1
6	IOD	B	1694	1/1	0.12	-1.13	52,52,52,52	1
6	IOD	B	1696	1/1	0.10	-1.14	64,64,64,64	1
6	IOD	A	1691	1/1	0.09	-1.18	65,65,65,65	1
6	IOD	C	1687	1/1	0.08	-1.25	63,63,63,63	1
6	IOD	D	1686	1/1	0.12	-1.31	54,54,54,54	1
6	IOD	A	1682	1/1	0.11	-1.41	55,55,55,55	1
6	IOD	C	1678	1/1	0.07	-1.43	52,52,52,52	1
6	IOD	C	1675	1/1	0.10	-1.44	55,55,55,55	1
6	IOD	D	1673	1/1	0.14	-1.45	77,77,77,77	1
6	IOD	D	1675	1/1	0.12	-1.49	76,76,76,76	1
6	IOD	C	1673	1/1	0.13	-1.52	50,50,50,50	1
6	IOD	A	1685	1/1	0.11	-1.59	55,55,55,55	1
6	IOD	C	1677	1/1	0.08	-1.59	78,78,78,78	1
6	IOD	D	1687	1/1	0.09	-1.82	59,59,59,59	1
6	IOD	A	1692	1/1	0.08	-1.86	48,48,48,48	1
6	IOD	D	1689	1/1	0.10	-1.87	54,54,54,54	1
6	IOD	B	1684	1/1	0.11	-2.99	66,66,66,66	1
6	IOD	A	1668	1/1	0.12	-3.72	62,62,62,62	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.