



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:43 am BST

PDB ID : 2W0Q  
Title : E. coli copper amine oxidase in complex with Xenon  
Authors : Pirrat, P.; Smith, M.A.; Pearson, A.R.; McPherson, M.J.; Phillips, S.E.V.  
Deposited on : 2008-08-20  
Resolution : 2.48 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

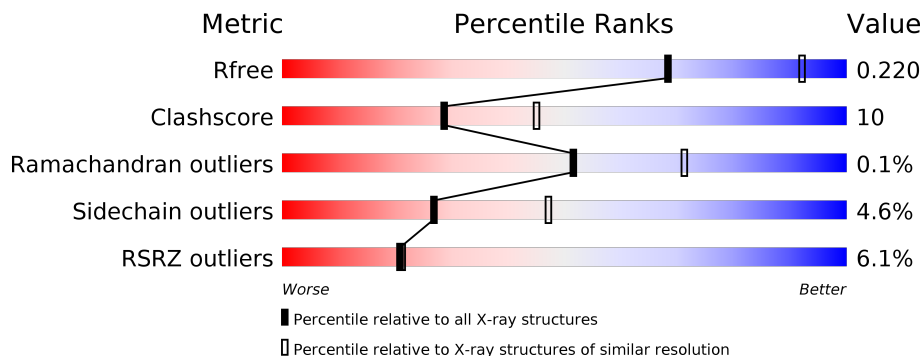
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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))
$R_{free}$	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	 4% 80% 17% ..
1	B	727	 8% 82% 16% ..

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
1	TPQ	A	466	-	-	X	-
1	TPQ	B	466	-	-	X	-
4	XE	A	904	-	-	X	-
4	XE	A	907	-	-	X	-
4	XE	A	908	-	-	X	-
4	XE	A	909	-	-	X	-
4	XE	B	905	-	-	X	-
4	XE	B	910	-	-	X	-
4	XE	B	911	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11947 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	719	5665	3602	965	1076	22	0	0	1
1	B	721	5683	3614	969	1078	22	0	0	1

- 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		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	Xe	0	0
			5	5		
4	A	6	Total	Xe	0	0
			6	6		

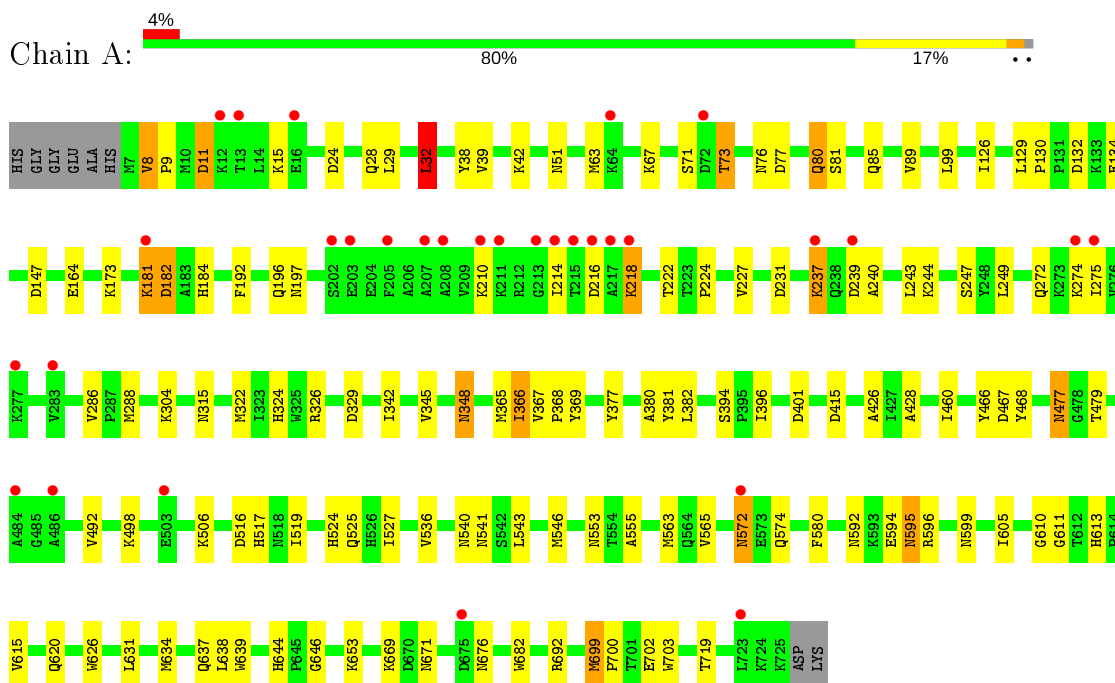
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	328	Total 328	O 328	0	0
5	B	254	Total 254	O 254	0	0

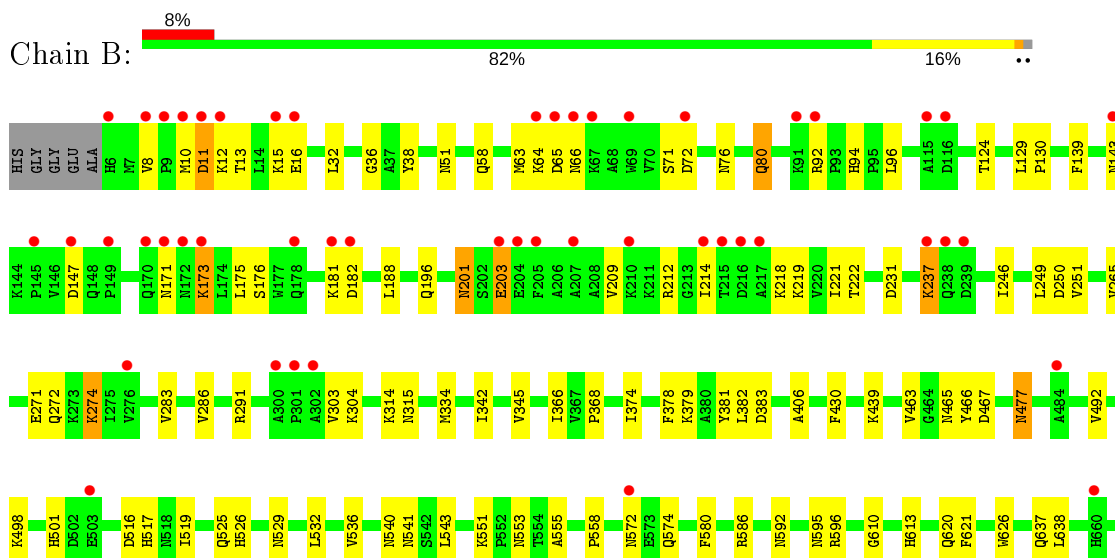
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: COPPER AMINE OXIDASE



- Molecule 1: COPPER AMINE OXIDASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.59Å 166.87Å 80.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.48 45.73 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.27-2.48) 98.1 (45.73-2.48)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.158 , 0.219 0.159 , 0.220	Depositor DCC
$R_{free}$ test set	3207 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, TPQ, CU, XE

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	0.91	3/5794 (0.1%)	0.86	6/7888 (0.1%)
1	B	0.83	0/5813	0.81	4/7912 (0.1%)
All	All	0.87	3/11607 (0.0%)	0.83	10/15800 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	MET	C-O	-18.67	0.87	1.23
1	A	699	MET	C-N	13.54	1.59	1.34
1	A	699	MET	CA-C	-12.63	1.20	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	MET	O-C-N	-16.87	89.05	121.10
1	A	699	MET	CA-C-O	15.12	151.86	120.10
1	B	692	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	B	692	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	586	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	415	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	692	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	B	586	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	692	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	32	LEU	CB-CG-CD1	5.69	120.67	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5665	0	5539	128	0
1	B	5683	0	5559	103	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	6	0	0	20	0
4	B	5	0	0	11	0
5	A	328	0	0	7	0
5	B	254	0	0	6	0
All	All	11947	0	11098	217	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 10.

All (217) 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:465:ASN:C	1:B:466:TPQ:H2	1.25	1.38
1:B:466:TPQ:C	1:B:467:ASP:N	1.94	1.31
1:A:605:ILE:HG13	4:A:909:XE:XE	2.10	1.30
1:A:28:GLN:HG3	5:A:2015:HOH:O	1.33	1.24
1:A:460:ILE:H	4:A:908:XE:XE	2.02	1.20
1:B:543:LEU:HD21	4:B:905:XE:XE	2.28	1.11
1:A:466:TPQ:HA	1:A:467:ASP:N	1.66	1.10
1:B:466:TPQ:CA	1:B:467:ASP:N	2.15	1.09
1:A:466:TPQ:CA	1:A:467:ASP:N	2.15	1.08
1:A:605:ILE:CG1	4:A:909:XE:XE	2.80	1.08
1:A:466:TPQ:C	1:A:467:ASP:N	2.19	1.06
1:B:638:LEU:CD2	4:B:905:XE:XE	2.87	1.01
1:B:182:ASP:HB2	5:B:2065:HOH:O	1.61	1.00
1:A:322:MET:SD	5:A:2039:HOH:O	2.21	0.98
1:A:572:ASN:ND2	1:A:671:ASN:HD21	1.62	0.97
1:B:466:TPQ:HA	1:B:467:ASP:N	1.78	0.97
1:B:94:HIS:HD2	1:B:96:LEU:H	1.13	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:PHE:H	1:B:637:GLN:HE21	1.13	0.94
1:A:315:ASN:HD21	1:B:304:LYS:H	1.14	0.94
1:B:638:LEU:HD21	4:B:905:XE:XE	2.47	0.92
1:A:574:GLN:H	1:A:671:ASN:ND2	1.68	0.92
1:A:304:LYS:H	1:B:315:ASN:HD21	0.99	0.91
1:B:466:TPQ:O	1:B:467:ASP:N	2.04	0.90
1:A:460:ILE:N	4:A:908:XE:XE	2.82	0.89
1:A:543:LEU:HD21	4:A:907:XE:XE	2.50	0.89
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.21	0.88
1:A:426:ALA:O	4:A:908:XE:XE	2.73	0.85
1:B:171:ASN:HB3	1:B:173:LYS:HZ1	1.42	0.83
1:B:12:LYS:O	1:B:16:GLU:HG2	1.82	0.79
1:B:540:ASN:HB3	1:B:676:ASN:ND2	1.98	0.78
1:B:638:LEU:HD23	4:B:905:XE:XE	2.61	0.77
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.66	0.77
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.66	0.76
1:A:536:VAL:H	1:A:541:ASN:HD21	1.33	0.75
1:B:580:PHE:H	1:B:637:GLN:NE2	1.84	0.75
1:A:381:TYR:HE1	4:A:904:XE:XE	2.47	0.75
1:B:381:TYR:HE2	4:B:911:XE:XE	2.49	0.74
1:A:466:TPQ:O	1:A:467:ASP:N	2.21	0.74
1:B:196:GLN:HE22	1:B:222:THR:H	1.35	0.74
1:A:38:TYR:H	1:A:51:ASN:HD21	1.35	0.72
1:A:572:ASN:HD22	1:A:671:ASN:HD21	1.37	0.72
1:A:580:PHE:H	1:A:637:GLN:HE21	1.35	0.71
1:A:638:LEU:HG	4:A:907:XE:XE	2.68	0.71
1:A:605:ILE:HG12	4:A:909:XE:XE	2.67	0.71
1:A:249:LEU:HD23	1:A:288:MET:CE	2.21	0.70
1:A:543:LEU:HD11	4:A:909:XE:XE	2.69	0.69
1:B:620:GLN:HE21	4:B:910:XE:XE	2.53	0.69
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.23	0.69
1:A:181:LYS:O	1:A:182:ASP:HB2	1.93	0.68
1:A:38:TYR:H	1:A:51:ASN:ND2	1.91	0.68
1:B:574:GLN:H	1:B:671:ASN:ND2	1.92	0.68
1:A:644:HIS:HD2	1:A:646:GLY:H	1.40	0.68
1:B:171:ASN:HB3	1:B:173:LYS:NZ	2.09	0.68
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.42	0.68
1:A:596:ARG:NH2	1:B:516:ASP:OD1	2.27	0.67
1:A:368:PRO:HG3	1:A:634:MET:CE	2.26	0.66
1:A:28:GLN:CG	5:A:2015:HOH:O	2.11	0.66
1:A:543:LEU:CD1	4:A:909:XE:XE	3.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.44	0.65
1:A:394:SER:O	4:A:908:XE:XE	2.93	0.65
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.62	0.65
1:A:76:ASN:HD22	1:A:80:GLN:HE21	1.45	0.64
1:B:379:LYS:HD3	5:B:2135:HOH:O	1.96	0.64
1:B:94:HIS:CD2	1:B:96:LEU:H	2.05	0.63
1:A:304:LYS:H	1:B:315:ASN:ND2	1.84	0.63
1:A:572:ASN:ND2	1:A:671:ASN:ND2	2.43	0.63
1:B:383:ASP:HB3	1:B:463:VAL:HG21	1.80	0.62
1:B:381:TYR:HE1	5:B:2135:HOH:O	1.83	0.62
1:B:553:ASN:ND2	1:B:555:ALA:H	1.98	0.62
1:A:638:LEU:CD2	4:A:907:XE:XE	3.26	0.62
1:B:214:ILE:HD11	1:B:286:VAL:HG21	1.81	0.61
1:A:315:ASN:ND2	1:B:304:LYS:H	1.93	0.61
1:B:525:GLN:NE2	1:B:620:GLN:H	1.99	0.60
1:B:525:GLN:HE22	1:B:620:GLN:H	1.50	0.60
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.83	0.60
1:A:477:ASN:HD22	1:A:477:ASN:C	2.04	0.60
1:B:498:LYS:O	1:B:517:HIS:HD2	1.83	0.60
1:A:477:ASN:HD22	1:A:479:THR:H	1.50	0.60
1:A:304:LYS:N	1:B:315:ASN:HD21	1.84	0.59
1:B:536:VAL:H	1:B:541:ASN:HD21	1.50	0.59
1:A:237:LYS:HE3	1:A:240:ALA:HB2	1.84	0.59
1:A:249:LEU:HD23	1:A:288:MET:HE3	1.84	0.59
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.21	0.59
1:A:546:MET:HE3	1:A:565:VAL:HG11	1.84	0.59
1:A:563:MET:HB3	4:B:910:XE:XE	2.80	0.59
1:B:465:ASN:C	1:B:466:TPQ:H	2.00	0.59
1:B:525:GLN:OE1	1:B:620:GLN:HG2	2.02	0.58
1:B:271:GLU:HG3	5:B:2087:HOH:O	2.03	0.58
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.84	0.58
1:A:580:PHE:H	1:A:637:GLN:NE2	2.01	0.58
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.38	0.58
1:A:580:PHE:N	1:A:637:GLN:HE21	2.02	0.58
1:A:644:HIS:CD2	1:A:646:GLY:H	2.20	0.58
1:B:237:LYS:NZ	1:B:237:LYS:HB3	2.19	0.57
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.38	0.57
1:A:595:ASN:ND2	1:A:599:ASN:H	2.02	0.57
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.40	0.57
1:A:477:ASN:ND2	1:A:479:THR:H	2.03	0.56
1:A:574:GLN:H	1:A:671:ASN:HD21	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:HE22	1:A:620:GLN:H	1.53	0.56
1:B:221:ILE:HD12	1:B:250:ASP:HB2	1.87	0.56
1:A:466:TPQ:C6	1:A:466:TPQ:N	2.67	0.55
1:B:38:TYR:H	1:B:51:ASN:ND2	2.02	0.55
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.26	0.55
1:B:196:GLN:NE2	1:B:222:THR:H	2.03	0.55
1:A:214:ILE:HD11	1:A:286:VAL:HG21	1.89	0.55
1:A:498:LYS:O	1:A:517:HIS:HD2	1.90	0.54
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.40	0.54
1:A:527:ILE:HD12	1:A:634:MET:HE3	1.89	0.54
1:A:466:TPQ:H	1:A:466:TPQ:C6	2.21	0.54
1:A:181:LYS:O	1:A:182:ASP:CB	2.57	0.53
1:B:638:LEU:CG	4:B:905:XE:XE	3.35	0.53
1:B:638:LEU:HG	4:B:905:XE:XE	2.86	0.53
1:A:381:TYR:CE1	4:A:904:XE:XE	3.35	0.53
1:B:212:ARG:HG2	1:B:283:VAL:HG22	1.90	0.53
1:A:572:ASN:C	1:A:572:ASN:HD22	2.13	0.53
1:A:77:ASP:O	1:A:81:SER:HB3	2.08	0.52
1:A:184:HIS:ND1	5:A:2083:HOH:O	2.34	0.52
1:B:38:TYR:H	1:B:51:ASN:HD21	1.57	0.52
1:A:572:ASN:ND2	1:A:572:ASN:C	2.63	0.52
1:B:11:ASP:OD2	1:B:15:LYS:HE3	2.10	0.52
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.75	0.52
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.93	0.51
1:A:553:ASN:ND2	1:A:555:ALA:H	2.09	0.51
1:B:381:TYR:CE2	4:B:911:XE:XE	3.37	0.51
1:A:638:LEU:CG	4:A:907:XE:XE	3.36	0.51
1:B:272:GLN:HE21	1:B:274:LYS:HE2	1.76	0.51
1:B:466:TPQ:N	1:B:466:TPQ:C6	2.73	0.51
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.93	0.51
1:B:171:ASN:CB	1:B:173:LYS:NZ	2.74	0.50
1:B:36:GLY:HA2	1:B:314:LYS:HE2	1.92	0.50
1:A:324:HIS:HD2	1:A:329:ASP:OD2	1.93	0.50
1:A:525:GLN:NE2	1:A:620:GLN:H	2.09	0.50
1:B:477:ASN:HD22	1:B:477:ASN:C	2.15	0.50
1:A:396:ILE:HG13	4:A:908:XE:XE	2.90	0.49
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.47	0.49
1:A:366:ILE:HD12	1:A:382:LEU:HG	1.95	0.49
1:A:11:ASP:OD1	1:A:15:LYS:NZ	2.43	0.49
1:B:175:LEU:O	1:B:176:SER:HB3	2.12	0.49
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HG22	1:A:345:VAL:CG2	2.43	0.49
1:B:94:HIS:HD2	1:B:96:LEU:N	1.96	0.48
1:A:29:LEU:HD12	1:A:42:LYS:HG2	1.95	0.48
1:A:24:ASP:OD1	1:A:24:ASP:C	2.52	0.48
1:B:10:MET:CE	1:B:32:LEU:HD21	2.43	0.48
1:B:466:TPQ:H	1:B:466:TPQ:C6	2.26	0.48
1:B:203:GLU:H	1:B:203:GLU:CD	2.18	0.47
1:A:574:GLN:H	1:A:671:ASN:HD22	1.55	0.47
1:A:272:GLN:HB3	1:A:274:LYS:HG2	1.96	0.47
1:A:382:LEU:HD12	5:A:2185:HOH:O	2.14	0.47
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.96	0.47
1:B:543:LEU:CD2	4:B:905:XE:XE	3.22	0.47
1:A:572:ASN:HD22	1:A:671:ASN:ND2	2.08	0.47
1:A:63:MET:HG3	5:A:2014:HOH:O	2.14	0.47
1:B:251:VAL:O	1:B:251:VAL:CG1	2.62	0.47
1:A:224:PRO:HB2	1:A:243:LEU:HD13	1.97	0.46
1:A:611:GLY:HA2	1:A:703:TRP:O	2.15	0.46
1:B:214:ILE:HG12	1:B:249:LEU:HD13	1.97	0.46
1:A:367:VAL:HG21	1:A:468:TYR:OH	2.16	0.46
1:A:216:ASP:OD1	1:A:218:LYS:HG3	2.16	0.46
1:A:231:ASP:HB2	1:A:626:TRP:CZ2	2.50	0.46
1:A:594:GLU:OE1	1:B:501:HIS:HE1	2.00	0.45
1:A:315:ASN:HD21	1:B:304:LYS:N	1.96	0.45
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.99	0.45
1:A:348:ASN:HD22	1:A:348:ASN:C	2.20	0.45
1:A:546:MET:CE	1:A:565:VAL:HG11	2.47	0.45
1:A:366:ILE:HD13	1:A:631:LEU:CD1	2.47	0.45
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.32	0.45
1:A:71:SER:OG	1:A:73:THR:HG22	2.17	0.45
1:A:460:ILE:HB	4:A:908:XE:XE	2.95	0.45
1:A:76:ASN:ND2	1:A:80:GLN:HE21	2.12	0.44
1:A:326:ARG:HH22	1:B:303:VAL:HG13	1.81	0.44
1:A:366:ILE:HD11	1:A:380:ALA:HB1	2.00	0.44
1:A:466:TPQ:O	1:A:467:ASP:CA	2.66	0.44
1:B:529:ASN:HA	1:B:683:MET:O	2.18	0.44
1:B:532:LEU:HD13	1:B:708:LEU:HD11	2.00	0.44
1:B:251:VAL:O	1:B:251:VAL:HG12	2.18	0.44
1:A:610:GLY:HA3	1:B:610:GLY:HA3	2.01	0.43
1:B:492:VAL:HG22	5:B:2186:HOH:O	2.19	0.43
1:A:466:TPQ:O2	5:A:2226:HOH:O	2.21	0.43
1:A:286:VAL:O	1:A:288:MET:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ASP:HB3	1:A:519:ILE:HB	2.00	0.43
1:A:32:LEU:HB2	1:A:39:VAL:HB	2.01	0.42
1:A:638:LEU:HD23	4:A:907:XE:XE	2.97	0.42
1:B:465:ASN:O	1:B:466:TPQ:N	2.38	0.42
1:A:196:GLN:HE22	1:A:222:THR:H	1.68	0.42
1:A:322:MET:HG2	4:A:903:XE:XE	2.98	0.42
1:B:526:HIS:O	1:B:686:GLY:HA3	2.20	0.42
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.35	0.42
1:A:477:ASN:C	1:A:477:ASN:ND2	2.72	0.42
1:B:551:LYS:HD2	1:B:551:LYS:HA	1.78	0.42
1:A:365:MET:HE3	1:A:365:MET:HB2	1.90	0.41
1:A:401:ASP:OD2	1:B:439:LYS:NZ	2.53	0.41
1:B:209:VAL:HG13	1:B:214:ILE:HB	2.02	0.41
1:B:342:ILE:HG22	1:B:345:VAL:CG2	2.50	0.41
1:B:717:THR:HB	1:B:720:LEU:HG	2.02	0.41
1:A:699:MET:HE3	1:A:702:GLU:HG3	2.02	0.41
1:B:201:ASN:HA	1:B:201:ASN:HD22	1.72	0.41
1:B:246:ILE:CD1	1:B:265:VAL:HG22	2.51	0.41
1:B:406:ALA:HA	1:B:430:PHE:HB3	2.03	0.41
1:A:192:PHE:HE1	4:A:901:XE:XE	2.82	0.41
1:A:76:ASN:HD22	1:A:80:GLN:NE2	2.15	0.41
1:A:129:LEU:HD12	1:A:130:PRO:HD2	2.02	0.41
1:A:164:GLU:OE2	1:A:653:LYS:HE3	2.21	0.41
1:A:536:VAL:H	1:A:541:ASN:ND2	2.10	0.41
1:B:139:PHE:C	1:B:139:PHE:CD1	2.93	0.41
1:B:124:THR:HG22	1:B:188:LEU:HD21	2.03	0.41
1:A:99:LEU:HD12	1:A:126:ILE:HG22	2.02	0.41
1:B:374:ILE:O	1:B:378:PHE:HE1	2.04	0.41
1:B:291:ARG:NE	5:B:2091:HOH:O	2.54	0.41
1:B:76:ASN:O	1:B:80:GLN:HB2	2.20	0.41
1:B:574:GLN:H	1:B:671:ASN:HD22	1.69	0.40
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.55	0.40
1:B:366:ILE:HD12	1:B:382:LEU:CD1	2.51	0.40
1:A:274:LYS:HE2	1:A:275:ILE:O	2.21	0.40
1:A:492:VAL:HB	1:A:519:ILE:HG23	2.03	0.40
1:A:699:MET:HA	1:A:700:PRO:HD3	1.81	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	715/727 (98%)	696 (97%)	18 (2%)	1 (0%)	51	71
1	B	718/727 (99%)	696 (97%)	21 (3%)	1 (0%)	51	71
All	All	1433/1454 (99%)	1392 (97%)	39 (3%)	2 (0%)	51	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	A	182	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/615 (99%)	580 (95%)	29 (5%)	25	45
1	B	610/615 (99%)	583 (96%)	27 (4%)	28	49
All	All	1219/1230 (99%)	1163 (95%)	56 (5%)	27	47

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

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ASP
1	A	32	LEU
1	A	67	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	73	THR
1	A	80	GLN
1	A	85	GLN
1	A	89	VAL
1	A	132	ASP
1	A	134	GLU
1	A	147	ASP
1	A	173	LYS
1	A	181	LYS
1	A	197	ASN
1	A	210	LYS
1	A	218	LYS
1	A	237	LYS
1	A	239	ASP
1	A	247	SER
1	A	348	ASN
1	A	366	ILE
1	A	477	ASN
1	A	506	LYS
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	615	VAL
1	A	669	LYS
1	A	719	THR
1	B	8	VAL
1	B	11	ASP
1	B	13	THR
1	B	58	GLN
1	B	63	MET
1	B	64	LYS
1	B	65	ASP
1	B	71	SER
1	B	72	ASP
1	B	80	GLN
1	B	92	ARG
1	B	143	ASN
1	B	147	ASP
1	B	173	LYS
1	B	181	LYS
1	B	201	ASN
1	B	203	GLU

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Mol	Chain	Res	Type
1	B	218	LYS
1	B	219	LYS
1	B	237	LYS
1	B	274	LYS
1	B	334	MET
1	B	477	ASN
1	B	595	ASN
1	B	613	HIS
1	B	676	ASN
1	B	725	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	80	GLN
1	A	97	ASN
1	A	170	GLN
1	A	178	GLN
1	A	196	GLN
1	A	197	ASN
1	A	200	ASN
1	A	272	GLN
1	A	315	ASN
1	A	324	HIS
1	A	327	ASN
1	A	348	ASN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	541	ASN
1	A	553	ASN
1	A	572	ASN
1	A	595	ASN
1	A	604	GLN
1	A	613	HIS
1	A	637	GLN
1	A	644	HIS
1	A	671	ASN
1	A	676	ASN

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Mol	Chain	Res	Type
1	B	51	ASN
1	B	94	HIS
1	B	97	ASN
1	B	170	GLN
1	B	196	GLN
1	B	197	ASN
1	B	200	ASN
1	B	201	ASN
1	B	238	GLN
1	B	263	ASN
1	B	272	GLN
1	B	307	GLN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	447	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	525	GLN
1	B	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	567	GLN
1	B	572	ASN
1	B	595	ASN
1	B	604	GLN
1	B	620	GLN
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	B	466	1	13,14,15	2.40	5 (38%)	15,19,21	1.77	5 (33%)
1	TPQ	A	466	1	13,14,15	2.44	4 (30%)	15,19,21	1.29	1 (6%)

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	B	466	1	-	4/5/22/24	0/1/1/1
1	TPQ	A	466	1	-	5/5/22/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	O2-C2	4.95	1.37	1.24
1	A	466	TPQ	O5-C5	4.88	1.37	1.24
1	B	466	TPQ	O5-C5	4.85	1.37	1.24
1	B	466	TPQ	O2-C2	4.44	1.36	1.24
1	A	466	TPQ	C3-C4	3.39	1.40	1.35
1	B	466	TPQ	C3-C4	3.26	1.40	1.35
1	B	466	TPQ	C6-C5	-2.67	1.37	1.44
1	A	466	TPQ	C6-C5	-2.15	1.38	1.44
1	B	466	TPQ	C3-C2	-2.12	1.39	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TPQ	C6-C1-C2	4.03	121.74	118.64
1	A	466	TPQ	C6-C1-C2	3.16	121.06	118.64
1	B	466	TPQ	O5-C5-C4	2.42	123.35	119.38
1	B	466	TPQ	C3-C4-C5	-2.27	118.91	121.26
1	B	466	TPQ	CB-C1-C2	2.26	122.61	118.57
1	B	466	TPQ	O5-C5-C6	-2.21	116.72	121.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	466	TPQ	N-CA-CB-C1
1	B	466	TPQ	C-CA-CB-C1
1	B	466	TPQ	O-C-CA-CB
1	A	466	TPQ	N-CA-CB-C1
1	A	466	TPQ	C-CA-CB-C1
1	A	466	TPQ	O-C-CA-CB
1	A	466	TPQ	C2-C1-CB-CA
1	A	466	TPQ	C6-C1-CB-CA
1	B	466	TPQ	C2-C1-CB-CA

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	TPQ	9	0
1	A	466	TPQ	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	466:TPQ	C	467:ASP	N	2.19
1	B	466:TPQ	C	467:ASP	N	1.94
1	B	465:ASN	C	466:TPQ	N	1.76
1	A	465:ASN	C	466:TPQ	N	1.62

## 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	718/727 (98%)	0.15	31 (4%) 35 37	19, 37, 60, 75	0
1	B	720/727 (99%)	0.28	56 (7%) 13 12	22, 40, 65, 78	0
All	All	1438/1454 (98%)	0.21	87 (6%) 21 21	19, 38, 62, 78	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	THR	6.6
1	B	215	THR	5.8
1	B	214	ILE	5.8
1	B	216	ASP	4.9
1	B	66	ASN	4.9
1	A	216	ASP	4.5
1	B	69	TRP	4.4
1	B	171	ASN	4.4
1	B	239	ASP	4.3
1	B	64	LYS	4.3
1	B	173	LYS	4.3
1	A	214	ILE	4.2
1	A	203	GLU	4.2
1	B	170	GLN	4.1
1	B	91	LYS	4.0
1	A	217	ALA	3.9
1	B	203	GLU	3.9
1	B	92	ARG	3.9
1	A	503	GLU	3.9
1	B	115	ALA	3.7
1	B	671	ASN	3.6
1	B	65	ASP	3.5
1	B	147	ASP	3.4
1	B	72	ASP	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	6	HIS	3.1
1	A	208	ALA	3.1
1	B	67	LYS	3.0
1	A	218	LYS	3.0
1	B	302	ALA	3.0
1	A	675	ASP	3.0
1	B	670	ASP	3.0
1	B	182	ASP	2.9
1	B	660	HIS	2.9
1	B	672	GLU	2.9
1	B	11	ASP	2.8
1	B	172	ASN	2.8
1	B	9	PRO	2.8
1	A	205	PHE	2.8
1	A	239	ASP	2.8
1	B	16	GLU	2.8
1	B	205	PHE	2.7
1	B	503	GLU	2.7
1	A	13	THR	2.7
1	A	181	LYS	2.6
1	A	64	LYS	2.6
1	B	484	ALA	2.6
1	B	12	LYS	2.6
1	B	181	LYS	2.6
1	B	10	MET	2.6
1	A	283	VAL	2.5
1	A	210	LYS	2.5
1	A	277	LYS	2.5
1	B	207	ALA	2.5
1	A	275	ILE	2.4
1	B	276	VAL	2.4
1	A	213	GLY	2.4
1	B	15	LYS	2.4
1	A	274	LYS	2.4
1	B	8	VAL	2.4
1	B	237	LYS	2.3
1	B	301	PRO	2.3
1	A	12	LYS	2.3
1	A	723	LEU	2.3
1	B	669	LYS	2.3
1	B	143	ASN	2.3
1	B	217	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	207	ALA	2.2
1	A	16	GLU	2.2
1	B	675	ASP	2.2
1	A	572	ASN	2.2
1	A	72	ASP	2.2
1	A	237	LYS	2.2
1	B	673	SER	2.2
1	B	238	GLN	2.2
1	B	300	ALA	2.2
1	A	486	ALA	2.1
1	A	484	ALA	2.1
1	A	202	SER	2.1
1	B	210	LYS	2.1
1	B	204	GLU	2.1
1	B	178	GLN	2.1
1	B	572	ASN	2.1
1	A	211	LYS	2.1
1	B	149	PRO	2.0
1	B	726	ASP	2.0
1	B	145	PRO	2.0
1	B	116	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	B	466	14/15	0.85	0.32	52,58,64,64	0
1	TPQ	A	466	14/15	0.90	0.25	52,60,63,63	0

## 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. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	XE	A	909	1/1	0.87	0.49	41,41,41,41	1
4	XE	B	910	1/1	0.90	0.33	46,46,46,46	1
4	XE	B	905	1/1	0.91	0.31	48,48,48,48	1
3	CA	B	803	1/1	0.94	0.23	77,77,77,77	0
4	XE	B	911	1/1	0.97	0.61	58,58,58,58	1
4	XE	A	907	1/1	0.97	0.15	49,49,49,49	1
4	XE	A	903	1/1	0.97	0.17	43,43,43,43	1
2	CU	B	801	1/1	0.97	0.12	45,45,45,45	0
4	XE	A	904	1/1	0.98	0.20	58,58,58,58	1
4	XE	B	906	1/1	0.98	0.17	57,57,57,57	1
4	XE	B	902	1/1	0.98	0.29	50,50,50,50	1
4	XE	A	901	1/1	0.99	0.10	58,58,58,58	1
3	CA	A	803	1/1	0.99	0.25	69,69,69,69	0
2	CU	A	801	1/1	0.99	0.14	47,47,47,47	0
4	XE	A	908	1/1	0.99	0.20	27,27,27,27	1
3	CA	B	802	1/1	1.00	0.07	31,31,31,31	0
3	CA	A	802	1/1	1.00	0.08	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.