Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 03:21 pm BST

PDB ID	:	2WOF
Title	:	EDTA treated E. coli copper amine oxidase
Authors	:	Smith, M.A.; Pirrat, P.; Pearson, A.R.; Knowles, P.F.; Phillips, S.E.V.; McPherson, M.J.
Deposited on	:	2009-07-23
Resolution	:	2.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

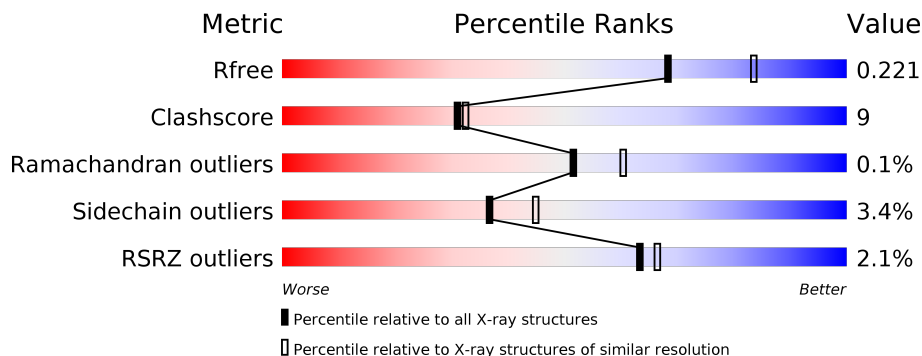|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	Percentile Ranks	Value
Rfree		0.221
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		3.4%
RSRZ outliers		2.1%

Worse ———— *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	% 83% 14% ••
1	B	727	3% 81% 16% ••

Full wwPDB X-ray Structure Validation Report

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12468 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 PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total 5691	C 3620	N 967	O 1081	S 23	0	4	1
1	B	721	Total 5711	C 3634	N 971	O 1082	S 24	0	4	1

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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	601	Total 601	O 601	0	0
4	B	459	Total 459	O 459	0	0

3 Residue-property plots (i)

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: PRIMARY AMINE OXIDASE
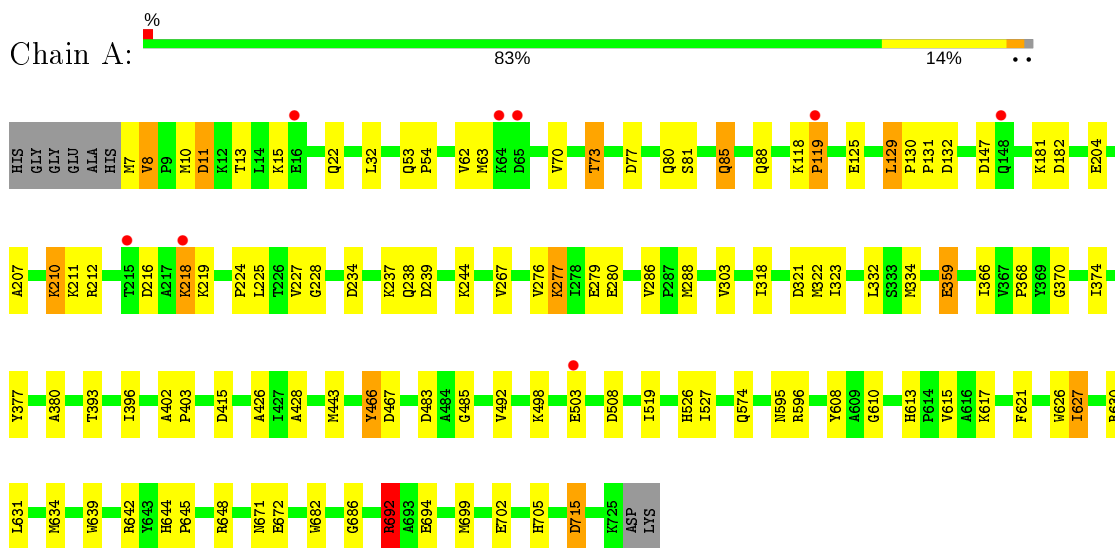
- Molecule 1: PRIMARY AMINE OXIDASE
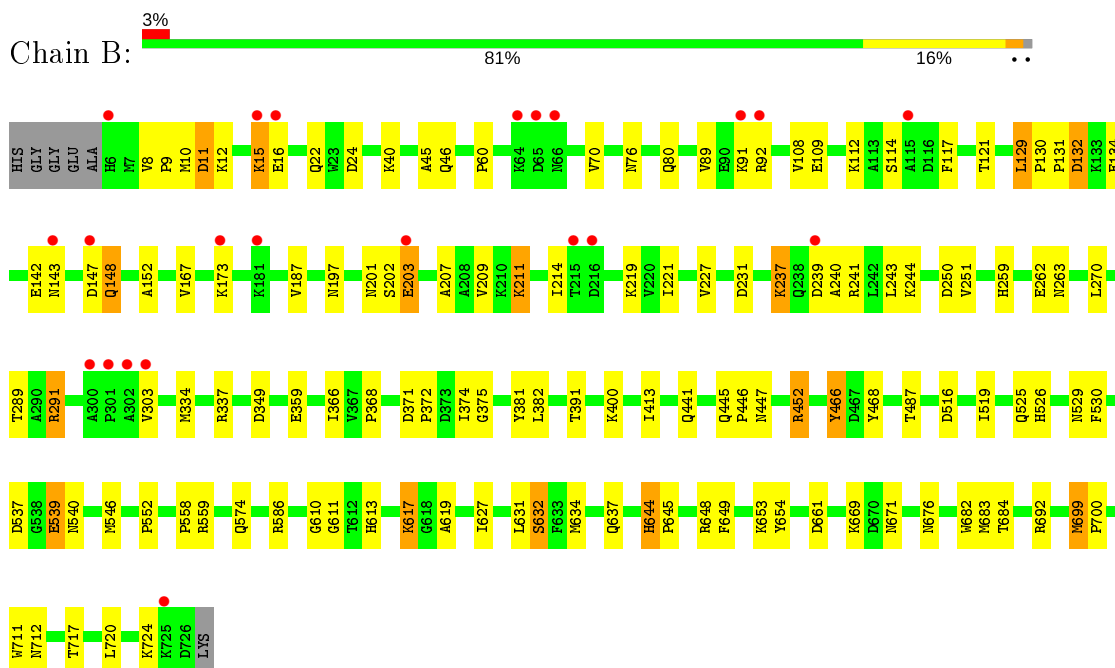
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.08Å 166.88Å 79.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.25 19.96 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.25) 99.8 (19.96-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.167 , 0.220 0.173 , 0.221	Depositor DCC
R_{free} test set	2947 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12468	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, TPQ, 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	0.93	2/5818 (0.0%)	0.88	7/7921 (0.1%)
1	B	0.93	1/5839 (0.0%)	0.86	4/7947 (0.1%)
All	All	0.93	3/11657 (0.0%)	0.87	11/15868 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	GLU	CB-CG	-6.21	1.40	1.52
1	B	109	GLU	CG-CD	5.37	1.60	1.51
1	A	426	ALA	CA-CB	5.02	1.62	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	586	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	234	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	467	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	415	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	452	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	119	PRO	C-N-CA	-5.46	108.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	692	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	715	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	537	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	349	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466[A]	TPQ	Mainchain
1	A	466[B]	TPQ	Mainchain
1	B	466[A]	TPQ	Mainchain
1	B	466[B]	TPQ	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5691	0	5565	99	0
1	B	5711	0	5588	110	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	601	0	0	15	0
4	B	459	0	0	20	0
All	All	12468	0	11153	206	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 9.

All (206) 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:A:237:LYS:NZ	1:A:239:ASP:HB2	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:MET:HG2	4:B:2112:HOH:O	1.54	1.06
1:B:8:VAL:CG2	1:B:9:PRO:HD2	1.87	1.03
1:A:132:ASP:HB3	4:A:2141:HOH:O	1.59	1.00
1:A:237:LYS:HZ3	1:A:239:ASP:HB2	1.16	1.00
1:B:221:ILE:CD1	1:B:250:ASP:HB2	1.93	0.98
1:B:700:PRO:HD2	4:B:2442:HOH:O	1.64	0.96
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.46	0.95
1:A:322:MET:HG2	4:A:2315:HOH:O	1.67	0.94
1:A:527:ILE:HD12	1:A:634:MET:HE3	1.50	0.94
1:A:10:MET:HE2	1:A:70:VAL:HG11	1.47	0.93
1:A:10:MET:CE	1:A:70:VAL:CG1	2.47	0.92
1:B:129:LEU:CD1	1:B:130:PRO:HD2	1.99	0.92
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.67	0.91
1:A:10:MET:HE2	1:A:70:VAL:CG1	2.00	0.91
1:B:129:LEU:HD13	1:B:130:PRO:HD2	1.54	0.88
1:B:221:ILE:HD13	1:B:250:ASP:HB2	1.52	0.88
1:B:203:GLU:H	1:B:203:GLU:CD	1.79	0.87
1:B:632:SER:OG	1:B:661:ASP:OD2	1.93	0.86
1:B:76:ASN:OD1	1:B:80:GLN:NE2	2.10	0.84
1:B:11:ASP:OD2	1:B:15:LYS:HE3	1.78	0.84
1:B:611:GLY:HA3	4:B:2396:HOH:O	1.78	0.83
1:A:527:ILE:HD12	1:A:634:MET:CE	2.06	0.83
1:A:322:MET:HE1	4:A:2058:HOH:O	1.80	0.82
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.63	0.81
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.81	0.80
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.63	0.80
1:B:219:LYS:HE3	4:B:2134:HOH:O	1.87	0.74
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.69	0.74
1:B:237:LYS:HE2	1:B:240:ALA:HB2	1.70	0.73
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.68	0.73
1:A:503:GLU:CD	1:A:503:GLU:H	1.93	0.71
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.20	0.71
1:A:10:MET:CE	1:A:70:VAL:HG11	2.16	0.70
1:A:527:ILE:CD1	1:A:634:MET:CE	2.70	0.70
1:B:8:VAL:HG22	1:B:9:PRO:CD	2.20	0.68
1:B:700:PRO:CD	4:B:2442:HOH:O	2.30	0.68
1:A:368:PRO:HG3	1:A:634:MET:CE	2.23	0.68
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.75	0.67
1:B:291:ARG:HD2	1:B:516:ASP:OD2	1.96	0.66
1:B:207:ALA:O	1:B:211:LYS:HD2	1.97	0.65
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:PRO:HB2	4:B:2442:HOH:O	1.98	0.64
1:A:237:LYS:NZ	1:A:239:ASP:CB	2.53	0.64
1:A:10:MET:CE	1:A:70:VAL:HG13	2.28	0.63
1:A:216:ASP:HB3	1:A:219:LYS:HD2	1.79	0.63
1:B:539:GLU:HG2	4:B:2354:HOH:O	1.98	0.63
1:B:644:HIS:ND1	1:B:645:PRO:HD2	2.14	0.62
1:A:286:VAL:CG1	1:A:288:MET:HE1	2.30	0.62
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.73	0.61
1:B:203:GLU:N	1:B:203:GLU:CD	2.50	0.60
1:A:228:GLY:HA3	4:A:2352:HOH:O	2.01	0.60
1:A:492:VAL:HB	1:A:519:ILE:HG23	1.84	0.59
1:A:359:GLU:CD	1:A:648:ARG:HH22	2.06	0.59
4:A:2427:HOH:O	1:B:400:LYS:HE3	2.03	0.58
1:A:238:GLN:HG3	1:A:238:GLN:O	2.04	0.58
1:B:359:GLU:CD	1:B:648:ARG:HH22	2.06	0.58
1:A:77:ASP:O	1:A:81:SER:HB3	2.03	0.58
1:B:221:ILE:CD1	1:B:250:ASP:CB	2.78	0.58
1:A:10:MET:HE3	1:A:70:VAL:CG1	2.33	0.57
1:B:40:LYS:HE2	4:B:2022:HOH:O	2.03	0.57
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.34	0.57
1:B:129:LEU:HD12	1:B:130:PRO:CD	2.34	0.57
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.69	0.56
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.70	0.56
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.85	0.56
1:A:119:PRO:HA	4:A:2118:HOH:O	2.05	0.55
1:B:382:LEU:N	1:B:382:LEU:HD12	2.23	0.54
1:B:337:ARG:HD3	1:B:649:PHE:CE1	2.42	0.54
1:A:10:MET:HE3	1:A:70:VAL:HG13	1.90	0.54
1:A:368:PRO:CG	1:A:634:MET:HE1	2.37	0.54
1:A:574:GLN:CG	1:A:671:ASN:CG	2.76	0.54
1:B:214:ILE:HD12	1:B:214:ILE:N	2.23	0.53
1:B:291:ARG:NE	4:B:2177:HOH:O	2.40	0.53
1:A:63:MET:HG3	4:A:2025:HOH:O	2.08	0.53
1:A:466[B]:TPQ:O5	1:A:699[B]:MET:HE1	2.09	0.53
1:A:574:GLN:HG3	1:A:671:ASN:CG	2.30	0.52
1:B:700:PRO:CB	4:B:2442:HOH:O	2.55	0.52
1:A:218:LYS:HD2	1:A:218:LYS:N	2.25	0.52
1:B:381:TYR:CD1	1:B:466[A]:TPQ:O5	2.64	0.52
1:B:466[B]:TPQ:HB2	1:B:468:TYR:CE2	2.44	0.52
1:B:711:TRP:O	1:B:712:ASN:HB2	2.10	0.52
1:B:45:ALA:O	1:B:60:PRO:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD12	1:A:130:PRO:HD2	1.93	0.51
1:A:7:MET:HE1	1:A:62:VAL:HG22	1.93	0.51
1:A:8:VAL:CG1	1:A:13:THR:OG1	2.59	0.51
1:A:11:ASP:O	1:A:15:LYS:HD2	2.09	0.51
1:A:224:PRO:C	1:A:225:LEU:HD12	2.32	0.50
1:B:552:PRO:HD2	4:B:2362:HOH:O	2.12	0.50
1:A:125:GLU:HA	4:A:2137:HOH:O	2.12	0.50
1:B:239:ASP:OD1	1:B:239:ASP:C	2.49	0.50
1:A:286:VAL:CG1	1:A:288:MET:CE	2.91	0.49
1:A:7:MET:CE	1:A:62:VAL:HG22	2.41	0.49
1:B:368:PRO:HD2	1:B:525:GLN:O	2.12	0.49
1:B:391:THR:HA	1:B:413:ILE:HD11	1.93	0.49
1:B:221:ILE:HD11	1:B:250:ASP:CB	2.40	0.49
1:A:286:VAL:HG11	1:A:288:MET:HE1	1.92	0.49
1:B:11:ASP:OD2	1:B:15:LYS:CE	2.56	0.49
1:A:73:THR:CG2	1:A:77:ASP:OD2	2.58	0.49
1:B:132:ASP:H	1:B:148:GLN:HE22	1.61	0.48
1:A:279:GLU:OE1	1:A:374:ILE:CD1	2.52	0.48
1:B:546:MET:HE2	4:B:2136:HOH:O	2.13	0.48
1:B:134:GLU:HG3	4:B:2037:HOH:O	2.13	0.48
1:B:12:LYS:HE2	1:B:16:GLU:OE2	2.14	0.48
1:B:237:LYS:HE3	1:B:237:LYS:HB2	1.54	0.48
1:B:540:ASN:HB3	1:B:676:ASN:OD1	2.13	0.48
1:B:46:GLN:HG2	1:B:60:PRO:HG3	1.96	0.48
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.49	0.48
1:A:7:MET:N	4:A:2001:HOH:O	2.47	0.48
1:B:129:LEU:HD12	1:B:129:LEU:C	2.33	0.48
1:A:366:ILE:HD13	1:A:631:LEU:CD1	2.44	0.47
1:A:210:LYS:O	1:A:211:LYS:C	2.52	0.47
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.28	0.47
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.96	0.47
1:B:241:ARG:HG2	1:B:270:LEU:HD12	1.97	0.47
1:B:187:VAL:HG22	1:B:243:LEU:HD21	1.97	0.47
1:A:85:GLN:HG2	1:A:88:GLN:HE22	1.79	0.47
1:A:8:VAL:HG13	1:A:13:THR:OG1	2.15	0.47
1:A:644:HIS:ND1	1:A:645:PRO:HD2	2.30	0.47
1:B:201:ASN:C	4:B:2132:HOH:O	2.53	0.47
1:A:118:LYS:HD2	1:A:119:PRO:HD2	1.97	0.46
1:B:129:LEU:HD12	1:B:130:PRO:N	2.31	0.46
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.97	0.46
1:B:366:ILE:CD1	1:B:631:LEU:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:HD12	1:B:631:LEU:HD13	1.97	0.46
1:A:503:GLU:CD	1:A:503:GLU:N	2.67	0.46
1:B:381:TYR:CE1	1:B:466[A]:TPQ:O5	2.69	0.46
1:B:231:ASP:CG	1:B:231:ASP:O	2.53	0.46
1:B:8:VAL:HG12	1:B:70:VAL:O	2.16	0.46
1:A:181:LYS:O	1:A:182:ASP:HB2	2.16	0.46
1:B:108:VAL:O	1:B:112:LYS:HG3	2.15	0.46
1:B:699[B]:MET:HA	1:B:700:PRO:HD3	1.82	0.46
1:A:237:LYS:HB3	4:A:2228:HOH:O	2.15	0.45
1:A:617:LYS:HD2	4:B:2381:HOH:O	2.16	0.45
1:B:142:GLU:O	1:B:143:ASN:HB3	2.17	0.45
1:A:692:ARG:HG3	1:A:694:GLU:OE1	2.17	0.45
1:A:212:ARG:HD3	4:A:2251:HOH:O	2.17	0.45
1:A:366:ILE:HD11	1:A:380:ALA:HB1	1.99	0.45
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.17	0.45
1:A:508:ASP:OD1	4:A:2456:HOH:O	2.21	0.45
1:A:22:GLN:NE2	4:A:2016:HOH:O	2.40	0.44
1:A:610:GLY:HA3	1:B:610:GLY:HA3	1.99	0.44
1:B:644:HIS:C	1:B:644:HIS:ND1	2.69	0.44
1:A:526:HIS:O	1:A:686:GLY:HA2	2.17	0.44
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.99	0.44
1:B:371:ASP:OD1	1:B:372:PRO:HD2	2.17	0.44
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.88	0.44
1:B:466[B]:TPQ:C4	1:B:526:HIS:CE1	3.01	0.44
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.38	0.44
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.39	0.43
1:A:483:ASP:CG	1:A:705:HIS:HD1	2.21	0.43
1:B:374:ILE:HG13	1:B:375:GLY:N	2.32	0.43
1:B:546:MET:CE	4:B:2136:HOH:O	2.66	0.43
1:B:637:GLN:HA	1:B:684:THR:HB	2.00	0.43
1:B:92:ARG:HB3	4:B:2056:HOH:O	2.18	0.43
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.48	0.43
1:B:259:HIS:HE1	1:B:289:THR:O	2.01	0.43
1:B:627:ILE:HG22	4:B:2400:HOH:O	2.18	0.43
1:A:11:ASP:OD1	1:A:15:LYS:HE3	2.19	0.43
1:B:129:LEU:CD1	1:B:130:PRO:CD	2.82	0.43
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.19	0.43
1:B:539:GLU:H	1:B:539:GLU:HG3	1.21	0.43
1:B:619:ALA:HB2	1:B:634:MET:HB3	2.01	0.43
1:B:717:THR:HB	1:B:720:LEU:HG	2.01	0.43
1:A:366:ILE:HD11	1:A:627:ILE:HD11	2.01	0.43

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Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:MET:HG3	1:B:70:VAL:HG13	1.99	0.43
1:A:402:ALA:HB1	1:A:403:PRO:HD2	2.01	0.43
1:A:642:ARG:CD	1:A:672:GLU:HB2	2.49	0.43
1:B:262:GLU:O	1:B:263:ASN:HB2	2.17	0.42
1:B:445:GLN:HB3	1:B:446:PRO:HD2	2.01	0.42
1:B:466[B]:TPQ:H6	1:B:487:THR:O	2.18	0.42
1:B:529:ASN:HA	1:B:683:MET:O	2.19	0.42
1:B:644:HIS:ND1	1:B:645:PRO:CD	2.82	0.42
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.54	0.42
1:B:653:LYS:HG2	1:B:654:TYR:CE2	2.54	0.42
1:B:574:GLN:HB2	1:B:671:ASN:OD1	2.18	0.42
1:A:466[B]:TPQ:O5	1:A:699[B]:MET:CE	2.66	0.42
1:B:24:ASP:C	1:B:24:ASP:OD1	2.56	0.42
1:A:276:VAL:O	1:A:277:LYS:HB2	2.19	0.42
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.84	0.42
1:A:63:MET:HE2	4:A:2061:HOH:O	2.20	0.42
1:B:202:SER:N	4:B:2132:HOH:O	2.53	0.42
1:B:720:LEU:HA	1:B:720:LEU:HD23	1.88	0.42
1:A:321:ASP:HB3	1:A:332:LEU:O	2.20	0.42
1:A:626:TRP:O	1:A:630:ARG:HG3	2.20	0.42
1:B:251:VAL:O	1:B:251:VAL:CG1	2.68	0.42
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.54	0.41
1:A:204:GLU:O	1:A:207:ALA:HB3	2.19	0.41
1:A:227:VAL:HG12	1:A:244:LYS:HG3	2.03	0.41
1:A:286:VAL:HB	1:A:288:MET:CE	2.51	0.41
1:B:530:PHE:O	1:B:682:TRP:HA	2.20	0.41
1:A:322:MET:CE	4:A:2046:HOH:O	2.68	0.41
1:A:334:MET:CE	1:A:393:THR:OG1	2.68	0.41
1:B:452:ARG:HA	4:B:2314:HOH:O	2.20	0.41
1:A:485:GLY:HA2	1:A:702:GLU:O	2.20	0.41
1:A:130:PRO:HA	1:A:131:PRO:HD3	1.81	0.41
1:A:286:VAL:HG12	1:A:288:MET:CE	2.51	0.41
1:B:466[B]:TPQ:C4	1:B:526:HIS:HE1	2.34	0.41
1:A:216:ASP:CB	1:A:219:LYS:HZ3	2.34	0.40
1:B:117:PHE:CZ	1:B:121:THR:HB	2.55	0.40
1:B:617:LYS:HG3	1:B:617:LYS:H	1.54	0.40
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.81	0.40
1:B:152:ALA:HB3	1:B:167:VAL:HG22	2.04	0.40
1:A:244:LYS:HG2	1:A:267:VAL:HG22	2.04	0.40
1:A:318:ILE:HG12	1:A:323:ILE:HG12	2.04	0.40
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.47	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	719/727 (99%)	698 (97%)	20 (3%)	1 (0%)	51	60
1	B	721/727 (99%)	703 (98%)	18 (2%)	0	100	100
All	All	1440/1454 (99%)	1401 (97%)	38 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	LYS

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	612/615 (100%)	597 (98%)	15 (2%)	47	56
1	B	614/615 (100%)	585 (95%)	29 (5%)	26	29
All	All	1226/1230 (100%)	1182 (96%)	44 (4%)	37	42

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ASP

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Mol	Chain	Res	Type
1	A	32	LEU
1	A	73	THR
1	A	80	GLN
1	A	85	GLN
1	A	129	LEU
1	A	147	ASP
1	A	210	LYS
1	A	218	LYS
1	A	303	VAL
1	A	498	LYS
1	A	613	HIS
1	A	627	ILE
1	A	692	ARG
1	B	11	ASP
1	B	15	LYS
1	B	22[A]	GLN
1	B	22[B]	GLN
1	B	89	VAL
1	B	91	LYS
1	B	114	SER
1	B	129	LEU
1	B	132	ASP
1	B	147	ASP
1	B	148	GLN
1	B	173	LYS
1	B	197	ASN
1	B	203	GLU
1	B	211	LYS
1	B	237	LYS
1	B	291	ARG
1	B	303	VAL
1	B	334	MET
1	B	539	GLU
1	B	613	HIS
1	B	617	LYS
1	B	632	SER
1	B	644	HIS
1	B	669	LYS
1	B	692	ARG
1	B	699[A]	MET
1	B	699[B]	MET
1	B	724	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	ASN
1	B	80	GLN
1	B	148	GLN
1	B	201	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	466[A]	-	13,14,15	2.42	5 (38%)	15,19,21	2.45	6 (40%)
1	TPQ	B	466[B]	2	13,14,15	2.24	5 (38%)	15,19,21	1.41	1 (6%)
1	TPQ	A	466[B]	2	13,14,15	2.18	6 (46%)	15,19,21	1.51	2 (13%)
1	TPQ	B	466[A]	-	13,14,15	2.33	4 (30%)	15,19,21	1.94	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
1	TPQ	A	466[A]	-	-	2/5/22/24	0/1/1/1
1	TPQ	B	466[B]	2	-	2/5/22/24	0/1/1/1
1	TPQ	A	466[B]	2	-	1/5/22/24	0/1/1/1
1	TPQ	B	466[A]	-	-	1/5/22/24	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466[A]	TPQ	O2-C2	5.58	1.39	1.24
1	B	466[A]	TPQ	O2-C2	4.98	1.37	1.24
1	A	466[A]	TPQ	O5-C5	4.61	1.36	1.24
1	B	466[B]	TPQ	O2-C2	4.49	1.36	1.24
1	B	466[B]	TPQ	O5-C5	4.46	1.36	1.24
1	B	466[A]	TPQ	O5-C5	4.39	1.36	1.24
1	A	466[B]	TPQ	O5-C5	4.18	1.35	1.24
1	A	466[B]	TPQ	O2-C2	4.16	1.35	1.24
1	B	466[A]	TPQ	C3-C4	3.44	1.41	1.35
1	A	466[B]	TPQ	C3-C4	2.80	1.40	1.35
1	A	466[A]	TPQ	C3-C4	2.57	1.39	1.35
1	B	466[B]	TPQ	C3-C4	2.44	1.39	1.35
1	A	466[B]	TPQ	C6-C5	-2.42	1.38	1.44
1	B	466[B]	TPQ	C6-C5	-2.37	1.38	1.44
1	A	466[A]	TPQ	C6-C5	-2.35	1.38	1.44
1	B	466[A]	TPQ	C6-C5	-2.25	1.38	1.44
1	B	466[B]	TPQ	C3-C2	-2.14	1.38	1.44
1	A	466[A]	TPQ	C3-C2	-2.06	1.39	1.44
1	A	466[B]	TPQ	C3-C2	-2.06	1.39	1.44
1	A	466[B]	TPQ	C6-C1	2.00	1.39	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	466[A]	TPQ	CB-CA-C	-5.27	101.59	111.47
1	A	466[A]	TPQ	C6-C1-C2	5.06	122.53	118.64
1	A	466[A]	TPQ	CB-CA-C	-4.30	103.41	111.47
1	A	466[A]	TPQ	O5-C5-C4	4.26	126.36	119.38
1	B	466[A]	TPQ	C6-C1-C2	3.92	121.65	118.64
1	A	466[A]	TPQ	O5-C5-C6	-3.11	114.66	121.78
1	B	466[B]	TPQ	CB-CA-C	2.91	116.92	111.47
1	A	466[A]	TPQ	O4-C4-C5	2.69	123.85	117.75
1	B	466[A]	TPQ	C6-C5-C4	2.16	120.69	117.03
1	A	466[B]	TPQ	C6-C5-C4	2.16	120.69	117.03
1	A	466[B]	TPQ	CB-C1-C2	2.09	122.31	118.57
1	A	466[A]	TPQ	O4-C4-C3	-2.07	115.42	121.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

　　Full wwPDB X-ray Structure Validation Report　　

Mol	Chain	Res	Type	Atoms
1	A	466[A]	TPQ	N-CA-CB-C1
1	A	466[A]	TPQ	C-CA-CB-C1
1	B	466[B]	TPQ	C-CA-CB-C1
1	A	466[B]	TPQ	C-CA-CB-C1
1	B	466[A]	TPQ	N-CA-CB-C1
1	B	466[B]	TPQ	N-CA-CB-C1

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466[B]	TPQ	4	0
1	A	466[B]	TPQ	2	0
1	B	466[A]	TPQ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	718/727 (98%)	-0.44	8 (1%)	80	82	20, 32, 50, 62	0
1	B	720/727 (99%)	-0.27	22 (3%)	49	52	21, 35, 56, 67	0
All	All	1438/1454 (98%)	-0.35	30 (2%)	63	66	20, 33, 54, 67	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	ALA	5.0
1	B	65	ASP	4.8
1	B	301	PRO	4.8
1	B	215	THR	4.7
1	A	64	LYS	4.0
1	B	115	ALA	3.9
1	B	6	HIS	3.8
1	B	66	ASN	3.3
1	A	215	THR	3.3
1	B	91	LYS	3.1
1	A	65	ASP	3.0
1	A	148	GLN	3.0
1	B	64	LYS	3.0
1	B	725	LYS	2.9
1	B	300	ALA	2.7
1	B	239	ASP	2.7
1	B	92	ARG	2.7
1	B	16	GLU	2.7
1	B	181	LYS	2.7
1	A	503	GLU	2.5
1	B	203	GLU	2.5
1	B	147	ASP	2.5
1	B	143	ASN	2.4
1	A	119	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	ASP	2.2
1	A	16	GLU	2.2
1	A	218	LYS	2.1
1	B	15	LYS	2.1
1	B	173	LYS	2.1
1	B	303	VAL	2.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPQ	A	466[A]	14/15	0.93	0.16	33,37,42,45	11
1	TPQ	A	466[B]	14/15	0.93	0.16	33,36,39,42	11
1	TPQ	B	466[B]	14/15	0.96	0.12	30,36,43,43	11
1	TPQ	B	466[A]	14/15	0.96	0.12	30,34,40,45	11

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	A	1727	1/1	0.87	0.11	30,30,30,30	0
3	NA	B	1728	1/1	0.95	0.10	36,36,36,36	0
3	NA	B	1729	1/1	0.98	0.12	30,30,30,30	0
3	NA	A	1728	1/1	0.99	0.18	26,26,26,26	0
2	CU	A	1726	1/1	0.99	0.05	40,40,40,40	0
2	CU	B	1727	1/1	0.99	0.03	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.