wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 10:28 AM EST

PDB ID	:	1D6Z
Title	:	CRYSTAL STRUCTURE OF THE AEROBICALLY FREEZE TRAPPED RATE-DETERMINING CATALYTIC INTERMEDIATE OF E. COLI COPPER-CONTAINING AMINE OXIDASE.
Authors	:	Wilmot, C.M.; Hajdu, J.; McPherson, M.J.; Knowles, P.F.; Phillips, S.E.V.
Deposited on	:	1999-10-16
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

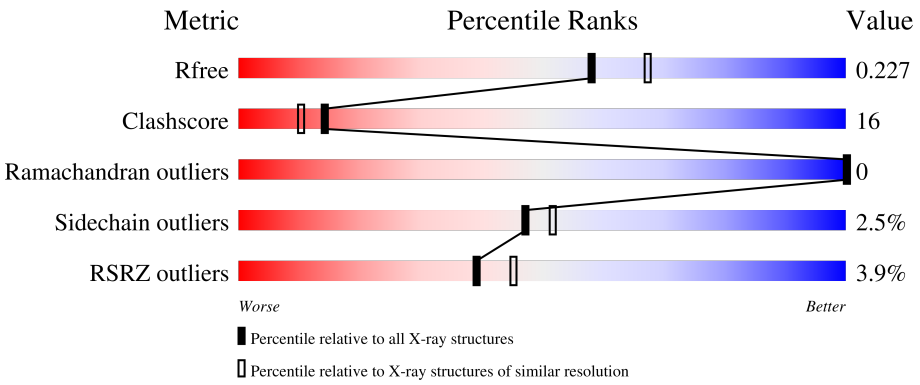
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of 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	3% 73% 23% • •
1	B	727	5% 74% 24% • •

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
5	PEO	A	2002	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12842 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	718	5664	3602	965	1075	22	0	0	0
1	B	720	5683	3614	970	1077	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TYY	TYR	modified residue	UNP P46883
B	466	TYY	TYR	modified residue	UNP P46883

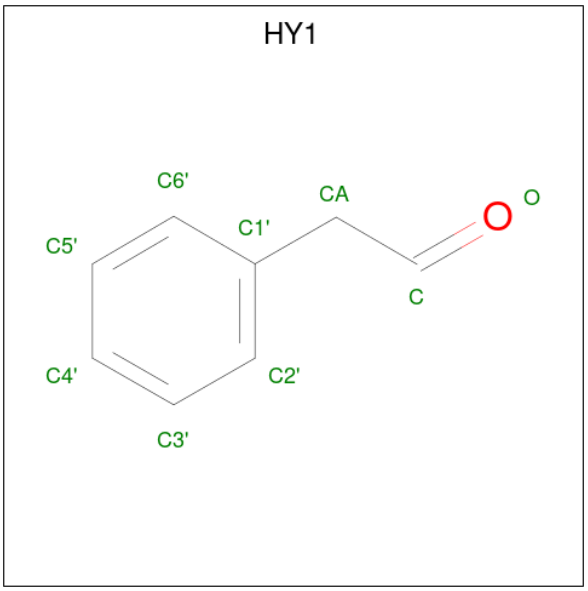
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

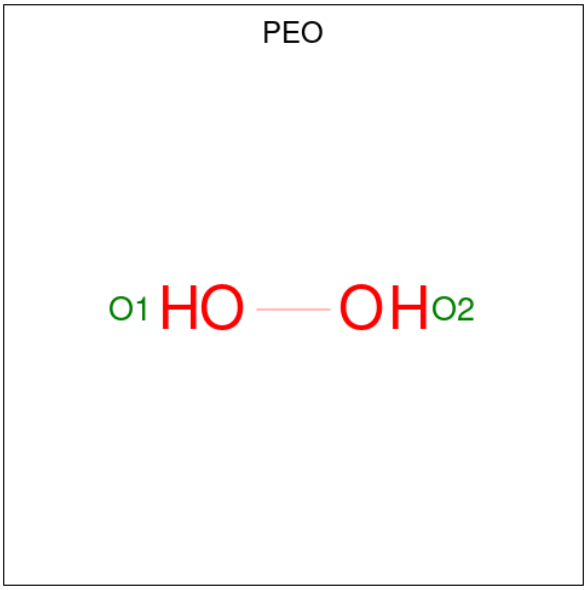
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is PHENYLACETALDEHYDE (three-letter code: HY1) (formula: C_8H_8O).



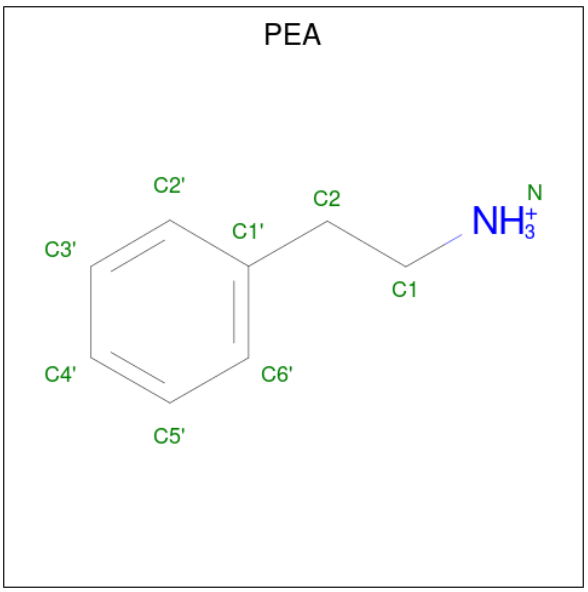
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 8 1	0	0
4	B	1	Total C O 9 8 1	0	0

- Molecule 5 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



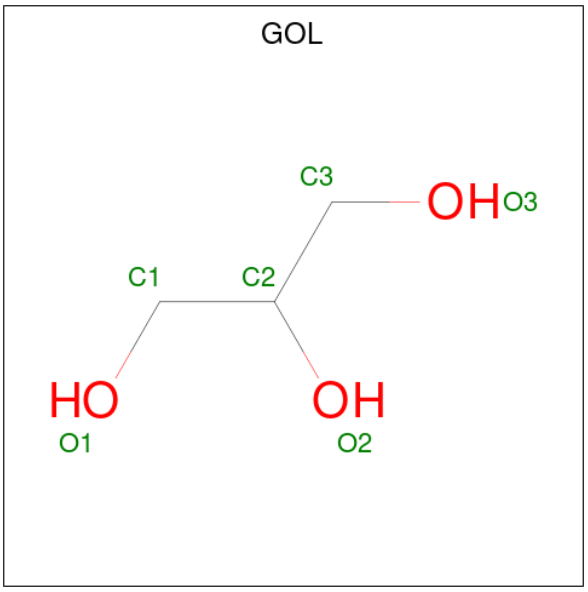
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is 2-PHENYLETHYLAMINE (three-letter code: PEA) (formula: $C_8H_{12}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
6	A	1	9	8	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	B	1	6	3	3	0	0

- Molecule 8 is water.

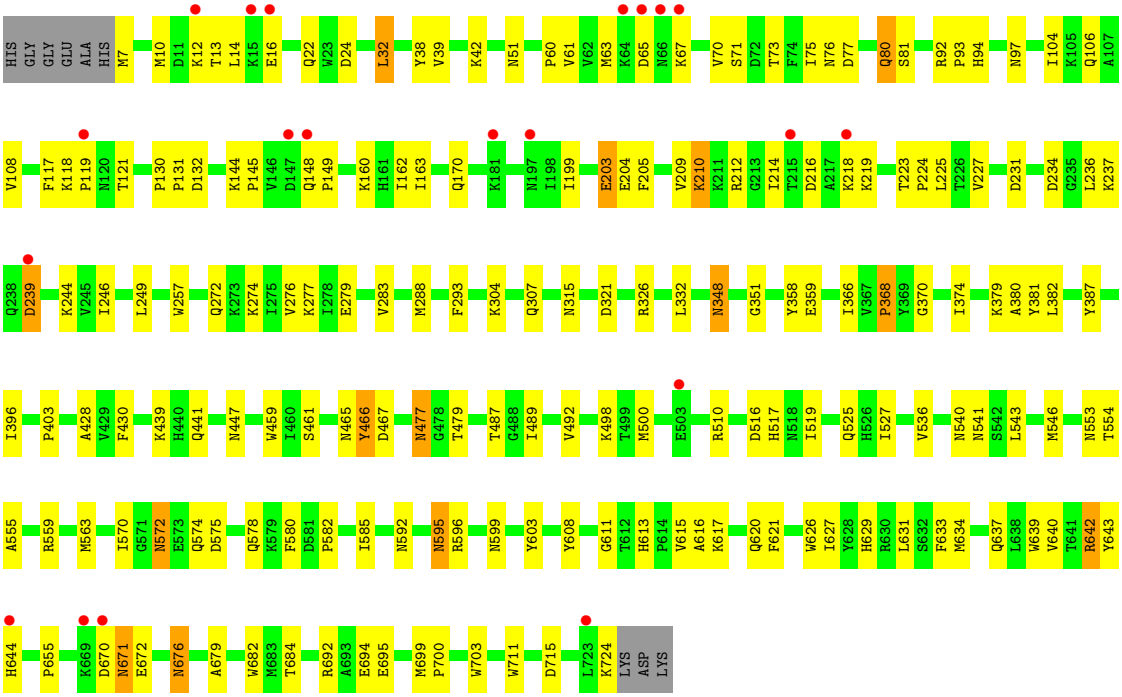
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	743	743	743	0	0
			Total	O		
8	B	703	703	703	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

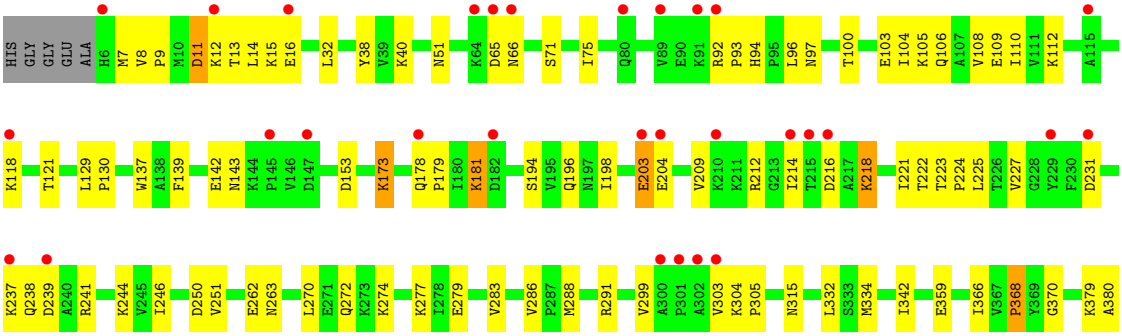
• Molecule 1: COPPER AMINE OXIDASE

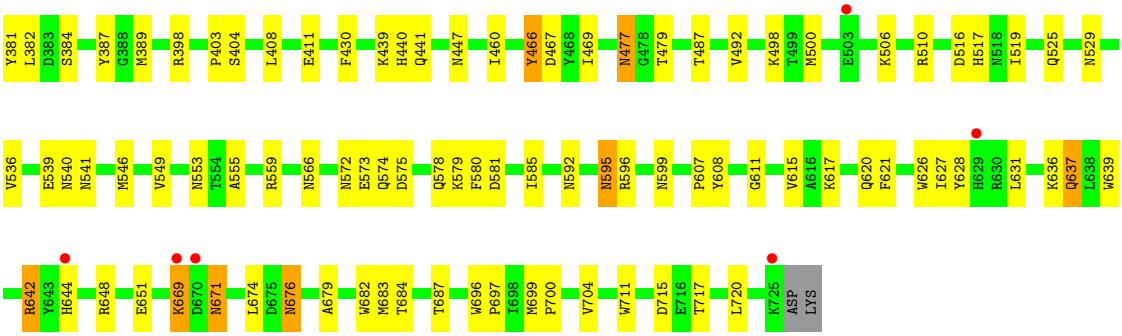
Chain A:



• Molecule 1: COPPER AMINE OXIDASE

Chain B:




Y381
L382
D383
S384
Y387
G388
M389
R398
P403
S404
L408
E411
F430
K439
H440
Q441
N447
I460
Y466
D467
Y468
I469
N477
G478
T479
T487
V492
K498
T499
M500
E503
K506
R510
D516
H517
N518
I519
Q525
N529
V536
E539
N540
N541
M546
V549
N553
T554
A555
R559
N566
N572
E573
Q574
D575
Q578
K579
F580
D581
I585
N592
N595
R596
N599
P607
Y608
G611
V615
A616
K617
Q620
F621
W626
I627
Y628
H629
R630
L631
K636
Q637
L638
W639
R642
Y643
H644
R648
E651
K669
D670
N671
L674
D675
N676
A679
W682
M683
T684
T687
W696
P697
I698
M699
P700
V704
W711
D715
E716
T717
L720
K725
ASP
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.24Å 166.48Å 79.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 23.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.10) 88.4 (23.58-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.237 0.185 , 0.227	Depositor DCC
R_{free} test set	3199 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 68.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12842	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PEO, GOL, CA, PEA, HY1, CU, TYY

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	0.32	0/5793	0.68	0/7886
1	B	0.32	0/5813	0.66	0/7912
All	All	0.32	0/11606	0.67	0/15798

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5664	0	5539	189	0
1	B	5683	0	5559	184	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	9	0	8	3	0
4	B	9	0	8	1	0
5	A	2	0	0	2	0
5	B	2	0	0	1	0
6	A	9	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	0	0
7	B	6	0	8	1	0
8	A	743	0	0	12	0
8	B	703	0	0	10	0
All	All	12842	0	11142	352	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 16.

The worst 5 of 352 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:181:LYS:H	1:B:181:LYS:HE2	0.98	1.05
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.22	1.01
1:A:642:ARG:HB2	1:A:642:ARG:HH11	1.26	0.97
1:B:181:LYS:HE2	1:B:181:LYS:N	1.84	0.93
1:B:181:LYS:H	1:B:181:LYS:CE	1.84	0.90

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%)	695 (97%)	20 (3%)	0	100	100
1	B	717/727 (99%)	696 (97%)	21 (3%)	0	100	100
All	All	1432/1454 (98%)	1391 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	594 (98%)	15 (2%)	47	52
1	B	611/615 (99%)	596 (98%)	15 (2%)	47	52
All	All	1220/1230 (99%)	1190 (98%)	30 (2%)	47	52

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	ASN
1	B	669	LYS
1	B	173	LYS
1	B	676	ASN
1	B	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	644	HIS
1	B	595	ASN
1	B	196	GLN
1	B	572	ASN
1	B	671	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)

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	TYY	A	466	1	11,14,15	2.44	4 (36%)	13,19,21	1.32	2 (15%)
1	TYY	B	466	1	11,14,15	2.39	5 (45%)	13,19,21	1.22	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYY	A	466	1	-	1/5/22/24	0/1/1/1
1	TYY	B	466	1	-	0/5/22/24	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TYY	CG-CD1	-6.28	1.39	1.49
1	B	466	TYY	CG-CD1	-6.24	1.39	1.49
1	A	466	TYY	CD2-CE2	-3.02	1.37	1.43
1	B	466	TYY	CD2-CE2	-2.63	1.38	1.43
1	A	466	TYY	CE1-CZ	2.33	1.39	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	TYY	CB-CA-C	-3.40	105.09	111.47
1	B	466	TYY	CB-CA-C	-2.82	106.17	111.47
1	B	466	TYY	CD2-CE2-CZ	2.27	120.31	117.91
1	A	466	TYY	CD2-CE2-CZ	2.17	120.20	117.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TYY	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466	TYY	2	0
1	B	466	TYY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	PEA	A	2003	-	8,9,9	1.60	3 (37%)	9,10,10	0.69	0
5	PEO	A	2002	2	1,1,1	1.60	0	-		
7	GOL	A	2004	-	5,5,5	0.51	0	5,5,5	0.51	0
4	HY1	A	2001	-	9,9,9	1.17	0	10,10,10	0.74	1 (10%)
4	HY1	B	3001	-	9,9,9	1.18	0	10,10,10	0.71	0
7	GOL	B	3003	-	5,5,5	0.36	0	5,5,5	0.45	0
5	PEO	B	3002	-	1,1,1	1.68	0	-		

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
6	PEA	A	2003	-	-	3/3/3/3	0/1/1/1
7	GOL	A	2004	-	-	2/4/4/4	-
4	HY1	A	2001	-	-	0/3/3/3	0/1/1/1
4	HY1	B	3001	-	-	0/3/3/3	0/1/1/1
7	GOL	B	3003	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2003	PEA	C3'-C2'	2.27	1.43	1.38
6	A	2003	PEA	C2'-C1'	2.20	1.43	1.38
6	A	2003	PEA	C3'-C4'	2.11	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	HY1	C1'-CA-C	-2.05	109.50	114.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2003	PEA	N-C1-C2-C1'
7	A	2004	GOL	C1-C2-C3-O3
7	A	2004	GOL	O2-C2-C3-O3
6	A	2003	PEA	C6'-C1'-C2-C1
6	A	2003	PEA	C2'-C1'-C2-C1

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2003	PEA	2	0
5	A	2002	PEO	2	0
4	A	2001	HY1	3	0
4	B	3001	HY1	1	0
7	B	3003	GOL	1	0
5	B	3002	PEO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	717/727 (98%)	-0.24	20 (2%)	53	59	15, 26, 46, 63	0
1	B	719/727 (98%)	-0.06	36 (5%)	28	34	16, 29, 52, 64	0
All	All	1436/1454 (98%)	-0.15	56 (3%)	39	45	15, 28, 50, 64	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	HIS	5.0
1	A	64	LYS	4.9
1	B	301	PRO	4.8
1	B	644	HIS	4.7
1	B	302	ALA	4.7

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	TYY	B	466	14/15	0.86	0.16	24,37,43,45	0
1	TYY	A	466	14/15	0.88	0.18	20,36,43,46	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
7	GOL	B	3003	6/6	0.79	0.21	48,50,51,52	0
4	HY1	B	3001	9/9	0.83	0.19	42,44,51,54	0
4	HY1	A	2001	9/9	0.85	0.18	45,46,48,50	0
7	GOL	A	2004	6/6	0.88	0.20	43,51,53,56	0
6	PEA	A	2003	9/9	0.89	0.13	26,29,31,31	0
5	PEO	A	2002	2/2	0.93	0.13	44,44,44,50	0
3	CA	B	803	1/1	0.93	0.14	64,64,64,64	0
5	PEO	B	3002	2/2	0.94	0.09	34,34,34,40	0
3	CA	A	803	1/1	0.95	0.16	60,60,60,60	0
3	CA	A	802	1/1	0.99	0.14	23,23,23,23	0
3	CA	B	802	1/1	0.99	0.09	28,28,28,28	0
2	CU	B	801	1/1	1.00	0.04	23,23,23,23	0
2	CU	A	801	1/1	1.00	0.04	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.