Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:05 PM GMT

PDB ID	:	4KFF
Title	:	Crystal structure of Hansenula polymorpha copper amine oxidase-1 reduced by methylamine at pH 8.5
Authors	:	Johnson, B.J.; Yukl, E.T.; Klema, V.J.; Wilmot, C.M.
Deposited on	:	2013-04-26
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

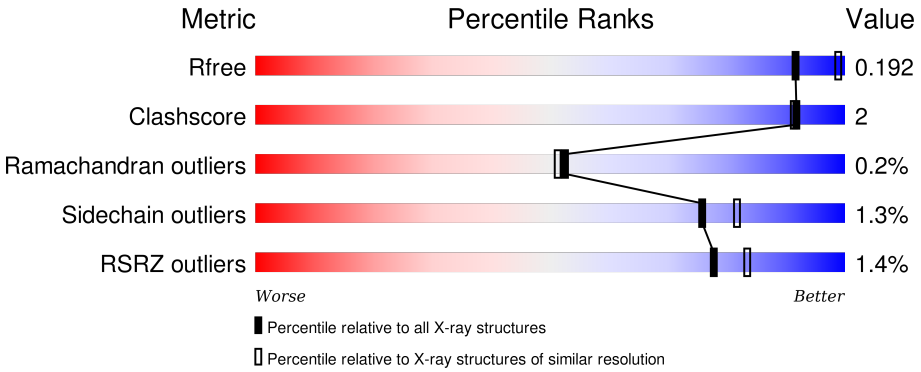
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

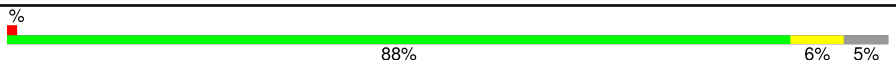
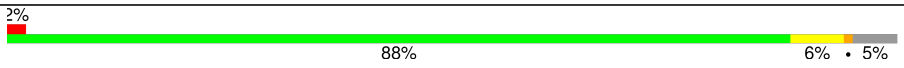
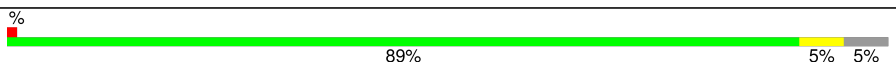
The reported resolution of this entry is 2.15 Å.

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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	692	
1	B	692	
1	C	692	

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
3	GOL	A	803	-	-	-	X
3	GOL	A	805	-	-	-	X
3	GOL	A	806	-	-	-	X
3	GOL	A	808	-	-	-	X
3	GOL	B	803	-	-	-	X
3	GOL	B	804	-	-	-	X
3	GOL	C	701	-	-	-	X
3	GOL	C	704	-	-	-	X
3	GOL	C	705	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16993 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.

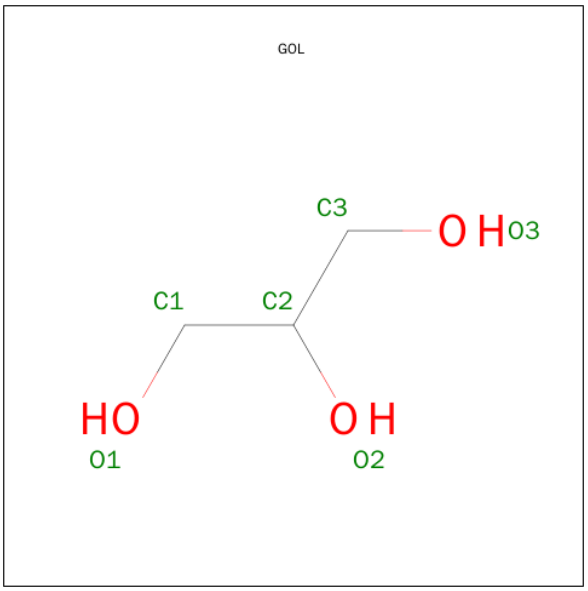
- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	S	0	2	0
			5217	3321	896	977	23			
1	B	657	Total	C	N	O	S	0	3	0
			5223	3325	896	979	23			
1	C	656	Total	C	N	O	S	0	5	0
			5223	3324	897	977	25			

- 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	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

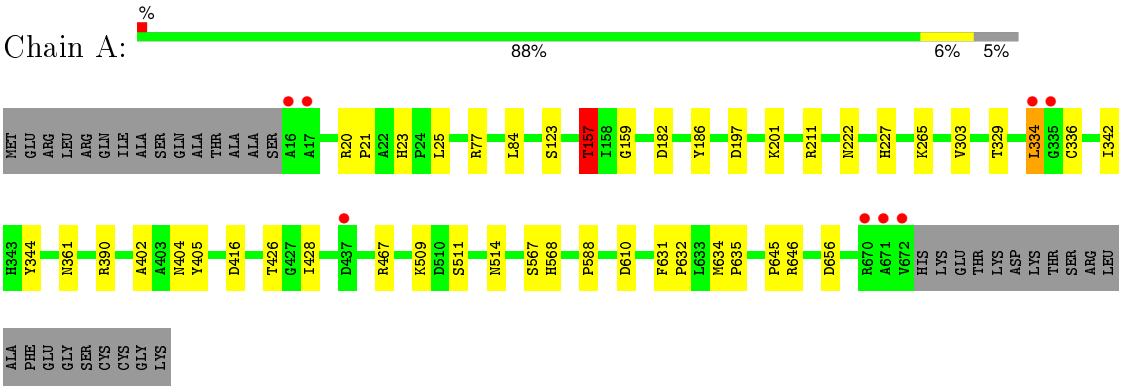
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	426	Total O 426 426	0	0
4	B	399	Total O 399 399	0	0
4	C	418	Total O 418 418	0	0

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 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.

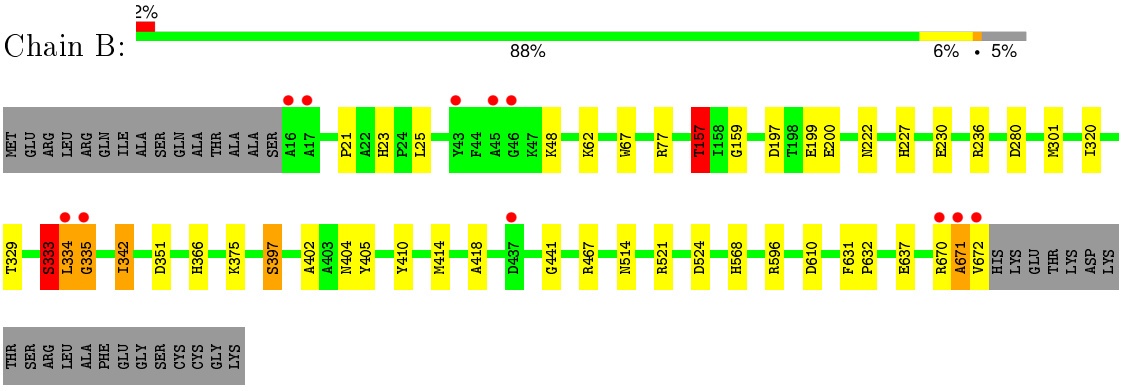
- Molecule 1: Peroxisomal primary amine oxidase

Chain A:



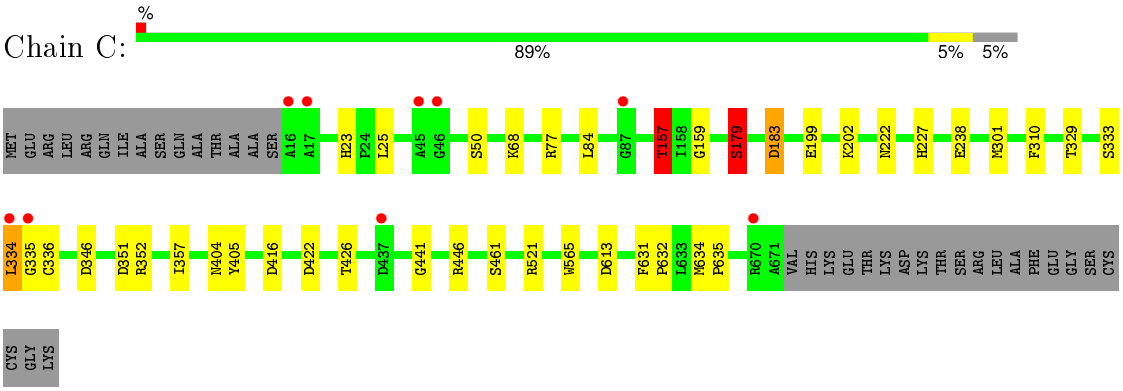
- Molecule 1: Peroxisomal primary amine oxidase

Chain B:



- Molecule 1: Peroxisomal primary amine oxidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.02Å 153.32Å 223.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.56 – 2.15 38.56 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.56-2.15) 99.9 (38.56-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.142 , 0.185 0.152 , 0.192	Depositor DCC
R_{free} test set	6489 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 128971 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16993	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TYY, 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	0.97	2/5344 (0.0%)	0.95	12/7274 (0.2%)
1	B	0.96	3/5353 (0.1%)	0.95	12/7286 (0.2%)
1	C	0.95	1/5359 (0.0%)	0.96	16/7294 (0.2%)
All	All	0.96	6/16056 (0.0%)	0.95	40/21854 (0.2%)

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	B	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	SER	CB-OG	-7.66	1.32	1.42
1	C	179	SER	CB-OG	-6.08	1.34	1.42
1	A	567	SER	CB-OG	-5.46	1.35	1.42
1	B	199	GLU	CG-CD	5.26	1.59	1.51
1	B	67	TRP	CB-CG	-5.10	1.41	1.50
1	A	511	SER	CB-OG	-5.06	1.35	1.42

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	521	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	C	446	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	656	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	390	ARG	NE-CZ-NH1	7.15	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	610	ASP	CB-CG-OD1	7.09	124.69	118.30
1	A	157	THR	CB-CA-C	-7.08	92.47	111.60
1	B	157	THR	CB-CA-C	-6.96	92.82	111.60
1	B	524	ASP	CB-CG-OD1	6.87	124.48	118.30
1	C	157	THR	CB-CA-C	-6.67	93.59	111.60
1	B	521	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	157	THR	N-CA-CB	6.51	122.68	110.30
1	B	596	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	157	THR	N-CA-CB	6.24	122.16	110.30
1	A	610	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	C	351	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	77	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	610	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	182	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	467	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	C	183	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	C	613	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	179	SER	CB-CA-C	-5.68	99.30	110.10
1	C	441	GLY	N-CA-C	-5.66	98.94	113.10
1	C	416	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	397	SER	CB-CA-C	-5.43	99.78	110.10
1	A	197	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	416	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	301	MET	CA-CB-CG	5.33	122.36	113.30
1	C	446	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	346	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	441	GLY	N-CA-C	-5.22	100.04	113.10
1	A	390	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	157	THR	N-CA-CB	5.17	120.12	110.30
1	C	613	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	236	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	197	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	351	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	422	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	336	CYS	CA-CB-SG	5.05	123.08	114.00
1	A	416	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	333	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	335	GLY	Peptide
1	B	671	ALA	Peptide

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	5217	0	5050	25	0
1	B	5223	0	5056	21	0
1	C	5223	0	5058	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	42	0	56	0	0
3	B	18	0	24	2	0
3	C	24	0	32	2	0
4	A	426	0	0	3	0
4	B	399	0	0	2	0
4	C	418	0	0	2	0
All	All	16993	0	15276	65	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 2.

All (65) 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:280:ASP:OD2	3:B:803:GOL:H12	1.69	0.92
1:C:23:HIS:HD2	1:C:25:LEU:H	1.25	0.83
1:B:23:HIS:HD2	1:B:25:LEU:H	1.24	0.82
1:A:23:HIS:HD2	1:A:25:LEU:H	1.28	0.81
1:A:157:THR:HB	1:A:159:GLY:H	1.51	0.75
1:A:405[B]:TYY:N5	4:A:957:HOH:O	2.23	0.72
1:C:199:GLU:HG3	4:C:1195:HOH:O	1.90	0.70
1:C:179:SER:HB2	1:C:183:ASP:OD2	1.96	0.65
1:B:157:THR:HB	1:B:159:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:PHE:CG	1:A:632:PRO:HA	2.34	0.61
1:C:157:THR:HB	1:C:159:GLY:H	1.66	0.61
1:A:402:ALA:O	1:A:405[B]:TYY:HD2	2.03	0.59
1:B:280:ASP:OD2	3:B:803:GOL:C1	2.48	0.57
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.88	0.56
1:A:157:THR:HB	1:A:159:GLY:N	2.20	0.55
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.43	0.54
1:B:631:PHE:CG	1:B:632:PRO:HA	2.43	0.54
1:A:344:TYR:HB3	1:A:361:ASN:HD22	1.73	0.54
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.39	0.53
1:A:334:LEU:HD21	4:A:1256:HOH:O	2.09	0.53
1:B:333:SER:HA	1:B:334:LEU:C	2.29	0.52
1:B:157:THR:HB	1:B:159:GLY:N	2.24	0.52
1:B:62:LYS:HE3	4:B:1271:HOH:O	2.09	0.52
1:C:631:PHE:CG	1:C:632:PRO:HA	2.45	0.52
1:A:404:ASN:HD21	1:A:405[B]:TYY:CZ	2.24	0.51
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.46	0.50
1:B:670:ARG:O	1:B:672:VAL:N	2.44	0.50
1:B:402:ALA:O	1:B:405[B]:TYY:HD2	2.13	0.48
1:C:199:GLU:CG	4:C:1195:HOH:O	2.55	0.48
1:B:23:HIS:CD2	1:B:25:LEU:H	2.15	0.48
1:A:404:ASN:HD21	1:A:405[B]:TYY:CE1	2.27	0.48
1:B:301:MET:HG3	1:B:320:ILE:HD12	1.96	0.47
1:A:303:VAL:HG23	4:A:1065:HOH:O	2.14	0.46
1:C:404:ASN:HD21	1:C:405[B]:TYY:CZ	2.28	0.45
1:B:342:ILE:HG22	1:B:366:HIS:HB3	1.98	0.45
1:A:645:PRO:O	1:A:646:ARG:HD2	2.17	0.45
1:B:514:ASN:OD1	1:B:568:HIS:HA	2.16	0.44
1:C:634:MET:HG2	1:C:635:PRO:O	2.17	0.44
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.33	0.44
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.53	0.44
1:A:157:THR:HG21	1:A:588:PRO:HB3	1.99	0.44
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.53	0.44
1:C:238:GLU:HA	1:C:238:GLU:OE2	2.16	0.44
1:A:123:SER:HB2	1:A:201:LYS:HE3	2.00	0.43
1:C:84:LEU:HD12	1:C:84:LEU:N	2.33	0.43
1:A:514:ASN:OD1	1:A:568:HIS:HA	2.18	0.43
1:A:405[A]:TYY:HD2	1:A:426:THR:O	2.18	0.43
1:B:404:ASN:HD21	1:B:405[B]:TYY:CZ	2.31	0.43
1:B:375:LYS:HE2	4:B:1278:HOH:O	2.19	0.43
1:C:68:LYS:HE3	3:C:703:GOL:H32	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.75	0.42
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.54	0.42
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.50	0.42
1:C:461:SER:HB2	1:C:565:TRP:CE3	2.55	0.42
1:C:405[A]:TYY:HD2	1:C:426:THR:O	2.19	0.41
1:C:334:LEU:HD23	1:C:335:GLY:H	1.86	0.41
1:A:342:ILE:HG21	1:A:344:TYR:CZ	2.56	0.41
1:C:50:SER:HB2	1:C:352:ARG:CD	2.51	0.41
1:B:397:SER:HG	1:B:410:TYR:HD1	1.64	0.41
1:A:84:LEU:HD12	1:A:84:LEU:N	2.36	0.40
1:A:186:TYR:CD2	1:A:428:ILE:HG21	2.55	0.40
1:C:310:PHE:CE1	3:C:704:GOL:H31	2.57	0.40
1:A:222:ASN:HB3	1:A:227:HIS:ND1	2.37	0.40
1:C:333:SER:HB2	1:C:336[B]:CYS:SG	2.62	0.40
1:A:634:MET:HG2	1:A:635:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	655/692 (95%)	631 (96%)	24 (4%)	0	100	100
1	B	656/692 (95%)	630 (96%)	23 (4%)	3 (0%)	34	26
1	C	657/692 (95%)	632 (96%)	25 (4%)	0	100	100
All	All	1968/2076 (95%)	1893 (96%)	72 (4%)	3 (0%)	52	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	SER
1	B	671	ALA

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Mol	Chain	Res	Type
1	B	335	GLY

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	566/593 (95%)	559 (99%)	7 (1%)	78	83
1	B	567/593 (96%)	558 (98%)	9 (2%)	70	76
1	C	568/593 (96%)	562 (99%)	6 (1%)	80	85
All	All	1701/1779 (96%)	1679 (99%)	22 (1%)	76	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	THR
1	A	211	ARG
1	A	265	LYS
1	A	329	THR
1	A	334	LEU
1	A	467	ARG
1	A	509	LYS
1	B	48	LYS
1	B	157	THR
1	B	200	GLU
1	B	230	GLU
1	B	329	THR
1	B	333	SER
1	B	334	LEU
1	B	342	ILE
1	B	637	GLU
1	C	157	THR
1	C	179	SER
1	C	202	LYS
1	C	329	THR
1	C	334	LEU

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Mol	Chain	Res	Type
1	C	357	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	70	GLN
1	A	361	ASN
1	B	23	HIS
1	B	66	GLN
1	B	361	ASN
1	B	382	ASN
1	C	23	HIS
1	C	70	GLN
1	C	361	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)

6 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	405[A]	-	12,14,15	1.38	3 (25%)	10,19,21	1.31	1 (10%)
1	TYY	A	405[B]	-	12,14,15	1.73	3 (25%)	10,19,21	1.98	3 (30%)
1	TYY	B	405[A]	-	12,14,15	0.93	0	10,19,21	1.10	0
1	TYY	B	405[B]	-	12,14,15	1.68	2 (16%)	10,19,21	1.89	4 (40%)
1	TYY	C	405[A]	-	12,14,15	1.35	1 (8%)	10,19,21	1.88	2 (20%)
1	TYY	C	405[B]	-	12,14,15	1.67	2 (16%)	10,19,21	2.09	3 (30%)

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	405[A]	-	-	0/4/22/24	0/1/1/1
1	TYY	A	405[B]	-	-	0/4/22/24	0/1/1/1
1	TYY	B	405[A]	-	-	0/4/22/24	0/1/1/1
1	TYY	B	405[B]	-	-	0/4/22/24	0/1/1/1
1	TYY	C	405[A]	-	-	0/4/22/24	0/1/1/1
1	TYY	C	405[B]	-	-	0/4/22/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405[B]	TYY	CD2-CE2	-4.71	1.33	1.42
1	B	405[B]	TYY	CD2-CE2	-4.40	1.34	1.42
1	C	405[B]	TYY	CD2-CE2	-3.98	1.35	1.42
1	A	405[A]	TYY	CD2-CE2	-2.61	1.37	1.42
1	A	405[B]	TYY	CE1-CD1	-2.21	1.38	1.44
1	A	405[A]	TYY	CE1-CZ	2.08	1.39	1.35
1	A	405[B]	TYY	CE1-CZ	2.21	1.39	1.35
1	B	405[B]	TYY	CE1-CZ	2.26	1.39	1.35
1	C	405[A]	TYY	CD2-CG	2.44	1.41	1.34
1	A	405[A]	TYY	CD2-CG	2.52	1.41	1.34
1	C	405[B]	TYY	CE1-CZ	2.56	1.39	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	405[A]	TYY	CB-CG-CD1	-3.47	112.91	118.33
1	C	405[A]	TYY	OZ-CD1-CG	-3.30	117.97	120.85
1	A	405[A]	TYY	OZ-CD1-CG	-2.86	118.35	120.85
1	B	405[B]	TYY	OZ-CD1-CG	-2.22	118.91	120.85
1	A	405[B]	TYY	O-C-CA	-2.20	119.75	125.49
1	B	405[B]	TYY	O-C-CA	-2.14	119.91	125.49
1	C	405[B]	TYY	CE1-CD1-CG	-2.13	116.70	118.30
1	B	405[B]	TYY	CD2-CG-CD1	2.12	119.94	118.44
1	A	405[B]	TYY	CB-CG-CD1	2.54	122.30	118.33
1	C	405[B]	TYY	CB-CG-CD1	2.96	122.94	118.33
1	B	405[B]	TYY	CB-CG-CD1	3.96	124.52	118.33
1	A	405[B]	TYY	CD2-CG-CD1	4.66	121.73	118.44
1	C	405[B]	TYY	CD2-CG-CD1	5.19	122.10	118.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405[A]	TYY	1	0
1	A	405[B]	TYY	4	0
1	B	405[B]	TYY	2	0
1	C	405[A]	TYY	1	0
1	C	405[B]	TYY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	GOL	A	802	-	5,5,5	0.39	0	5,5,5	0.62	0
3	GOL	A	803	-	5,5,5	1.04	0	5,5,5	1.76	2 (40%)
3	GOL	A	804	-	5,5,5	0.40	0	5,5,5	0.63	0
3	GOL	A	805	-	5,5,5	0.79	0	5,5,5	1.19	0
3	GOL	A	806	-	5,5,5	0.46	0	5,5,5	1.22	0
3	GOL	A	807	-	5,5,5	0.52	0	5,5,5	1.13	0
3	GOL	A	808	-	5,5,5	0.52	0	5,5,5	0.97	0
3	GOL	B	802	-	5,5,5	0.53	0	5,5,5	1.08	1 (20%)
3	GOL	B	803	-	5,5,5	0.59	0	5,5,5	1.51	1 (20%)
3	GOL	B	804	-	5,5,5	0.45	0	5,5,5	1.17	0
3	GOL	C	701	-	5,5,5	0.40	0	5,5,5	1.71	2 (40%)
3	GOL	C	703	-	5,5,5	0.20	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	C	704	-	5,5,5	0.41	0	5,5,5	0.74	0
3	GOL	C	705	-	5,5,5	0.16	0	5,5,5	1.29	1 (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
3	GOL	A	802	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
3	GOL	A	805	-	-	0/4/4/4	0/0/0/0
3	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	GOL	A	807	-	-	0/4/4/4	0/0/0/0
3	GOL	A	808	-	-	0/4/4/4	0/0/0/0
3	GOL	B	802	-	-	0/4/4/4	0/0/0/0
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
3	GOL	B	804	-	-	0/4/4/4	0/0/0/0
3	GOL	C	701	-	-	0/4/4/4	0/0/0/0
3	GOL	C	703	-	-	0/4/4/4	0/0/0/0
3	GOL	C	704	-	-	0/4/4/4	0/0/0/0
3	GOL	C	705	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	701	GOL	O1-C1-C2	-2.89	96.15	110.18
3	C	705	GOL	O3-C3-C2	-2.59	97.63	110.18
3	B	802	GOL	O1-C1-C2	-2.23	99.37	110.18
3	C	701	GOL	O2-C2-C1	-2.10	99.03	108.65
3	A	803	GOL	O2-C2-C1	-2.09	99.05	108.65
3	B	803	GOL	C3-C2-C1	-2.07	103.01	111.12
3	A	803	GOL	C3-C2-C1	3.11	123.31	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	GOL	2	0
3	C	703	GOL	1	0
3	C	704	GOL	1	0

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^{th} 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	656/692 (94%)	-0.57	8 (1%) 81 85	13, 19, 36, 80	0
1	B	656/692 (94%)	-0.46	11 (1%) 73 80	13, 20, 37, 88	0
1	C	655/692 (94%)	-0.43	9 (1%) 78 83	13, 20, 38, 62	0
All	All	1967/2076 (94%)	-0.49	28 (1%) 78 83	13, 20, 38, 88	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	VAL	9.3
1	B	335	GLY	6.3
1	C	16	ALA	5.0
1	A	16	ALA	4.5
1	A	672	VAL	4.5
1	A	671	ALA	4.5
1	B	16	ALA	4.5
1	A	335	GLY	3.9
1	C	335	GLY	3.8
1	A	17	ALA	3.8
1	A	334	LEU	3.5
1	B	46	GLY	3.5
1	B	670	ARG	3.2
1	B	334	LEU	3.0
1	C	670	ARG	2.9
1	B	45	ALA	2.7
1	C	334	LEU	2.7
1	B	671	ALA	2.7
1	C	45	ALA	2.7
1	B	17	ALA	2.6
1	B	437	ASP	2.6
1	C	46	GLY	2.6
1	A	437	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	437	ASP	2.5
1	A	670	ARG	2.5
1	C	17	ALA	2.2
1	C	87	GLY	2.1
1	B	43	TYR	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. 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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	TYY	A	405[B]	14/15	0.97	0.18	-	15,17,18,18	11
1	TYY	B	405[B]	14/15	0.94	0.25	-	13,16,17,18	11
1	TYY	C	405[A]	14/15	0.95	0.23	-	12,16,17,17	11
1	TYY	A	405[A]	14/15	0.97	0.18	-	16,18,20,22	11
1	TYY	C	405[B]	14/15	0.95	0.23	-	15,17,18,18	11
1	TYY	B	405[A]	14/15	0.94	0.25	-	16,17,19,20	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. 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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	A	806	6/6	0.91	0.29	10.91	39,45,46,47	0
3	GOL	B	804	6/6	0.89	0.27	10.14	46,49,51,52	0
3	GOL	C	701	6/6	0.92	0.21	8.48	43,46,49,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	B	803	6/6	0.91	0.18	3.90	35,39,41,41	0
3	GOL	C	704	6/6	0.95	0.14	3.69	40,41,44,44	0
3	GOL	A	803	6/6	0.81	0.17	3.50	36,45,48,61	0
3	GOL	A	805	6/6	0.91	0.15	3.00	34,44,47,48	0
3	GOL	A	808	6/6	0.96	0.10	2.41	23,34,37,41	0
3	GOL	C	705	6/6	0.91	0.17	2.16	38,51,55,64	0
3	GOL	C	703	6/6	0.96	0.10	1.55	29,30,37,46	0
3	GOL	A	802	6/6	0.91	0.17	1.42	31,33,35,39	0
3	GOL	B	802	6/6	0.89	0.13	0.89	30,32,35,35	0
2	CU	B	801	1/1	1.00	0.08	-	18,18,18,18	0
3	GOL	A	807	6/6	0.84	0.20	-	55,58,61,63	0
2	CU	A	801	1/1	1.00	0.08	-	19,19,19,19	0
2	CU	C	702	1/1	1.00	0.08	-	18,18,18,18	0
3	GOL	A	804	6/6	0.92	0.17	-	35,41,43,51	0

6.5 Other polymers (i)

There are no such residues in this entry.