



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:05 PM GMT

PDB ID : 4KFE  
Title : Crystal structure of Hansenula polymorpha copper amine oxidase-1 reduced by methylamine at pH 7.0  
Authors : Johnson, B.J.; Yukl, E.T.; Klema, V.J.; Wilmot, C.M.  
Deposited on : 2013-04-26  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

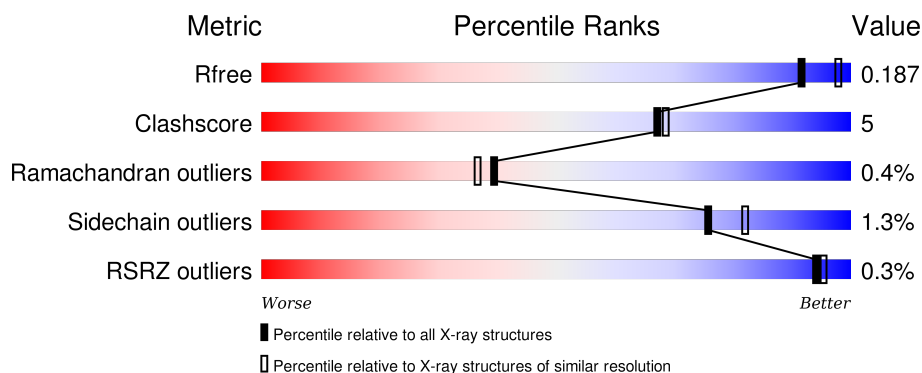
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	692	<div> <div>85%</div> <div>9% • 5%</div> </div>
1	B	692	<div> <div>85%</div> <div>9% 5%</div> </div>
1	C	692	<div> <div>86%</div> <div>8% 5%</div> </div>
1	D	692	<div> <div>86%</div> <div>8% 5%</div> </div>
1	E	692	<div> <div>85%</div> <div>10% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	692	 88%7%5%

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	PEO	B	802	-	-	-	X
3	PEO	C	802	-	X	-	X
3	PEO	D	701	-	X	-	-
3	PEO	E	802	-	-	-	X
3	PEO	F	802	-	X	-	X
4	FOR	A	803	-	-	-	X
4	FOR	B	803	-	-	-	X
4	FOR	D	702	-	-	-	X
5	GOL	A	804	-	-	-	X
5	GOL	A	807	-	-	-	X
5	GOL	A	809	-	-	-	X
5	GOL	A	810	-	-	-	X
5	GOL	A	813	-	-	-	X
5	GOL	A	814	-	-	-	X
5	GOL	A	815	-	-	-	X
5	GOL	A	816	-	-	-	X
5	GOL	B	805	-	-	-	X
5	GOL	B	806	-	-	-	X
5	GOL	B	808	-	-	-	X
5	GOL	B	809	-	-	-	X
5	GOL	B	810	-	-	-	X
5	GOL	B	811	-	-	-	X
5	GOL	C	803	-	-	-	X
5	GOL	C	804	-	-	-	X
5	GOL	C	806	-	-	-	X
5	GOL	C	807	-	-	-	X
5	GOL	C	809	-	-	-	X
5	GOL	C	810	-	-	-	X
5	GOL	D	704	-	-	-	X
5	GOL	D	706	-	-	-	X
5	GOL	D	709	-	-	-	X
5	GOL	D	711	-	-	X	X
5	GOL	D	712	-	-	-	X
5	GOL	E	804	-	-	-	X
5	GOL	E	805	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	E	806	-	-	-	X
5	GOL	E	807	-	-	-	X
5	GOL	F	803	-	-	-	X
5	GOL	F	804	-	-	-	X
5	GOL	F	805	-	-	-	X
5	GOL	F	806	-	-	-	X
5	GOL	F	807	-	-	-	X
5	GOL	F	808	-	-	-	X
5	GOL	F	810	-	-	-	X
5	GOL	F	811	-	-	-	X
5	GOL	F	812	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 36172 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.

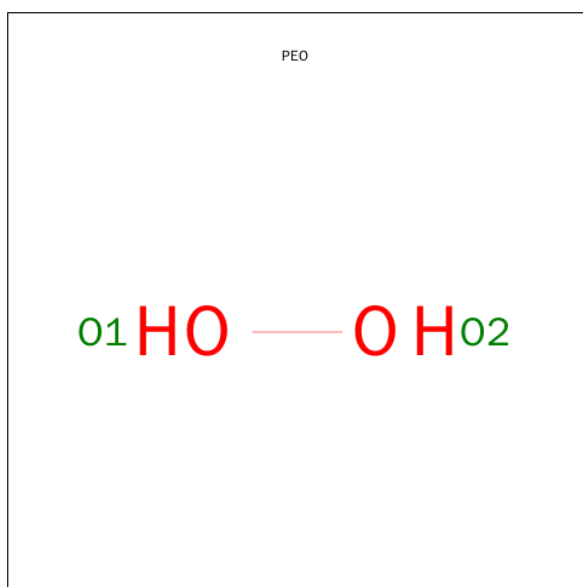
- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	0	5	0
			5249	3338	904	983	24			
1	B	658	Total	C	N	O	S	0	4	0
			5230	3328	898	980	24			
1	C	656	Total	C	N	O	S	0	10	0
			5253	3347	900	981	25			
1	D	656	Total	C	N	O	S	0	9	0
			5245	3338	899	984	24			
1	E	656	Total	C	N	O	S	0	5	0
			5223	3326	896	977	24			
1	F	656	Total	C	N	O	S	0	7	0
			5236	3334	898	979	25			

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

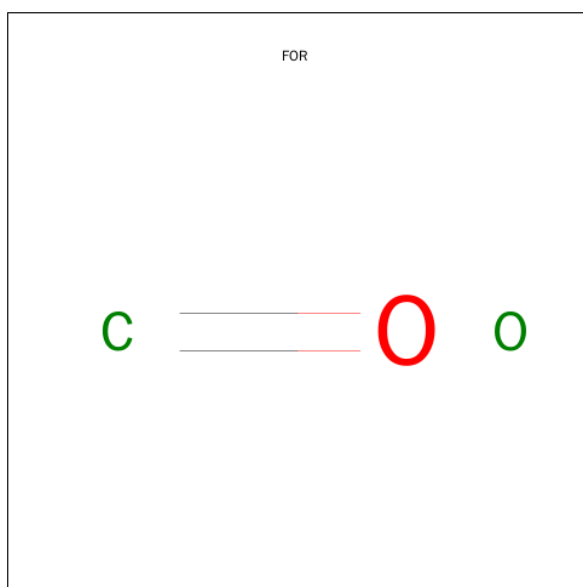
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H<sub>2</sub>O<sub>2</sub>).



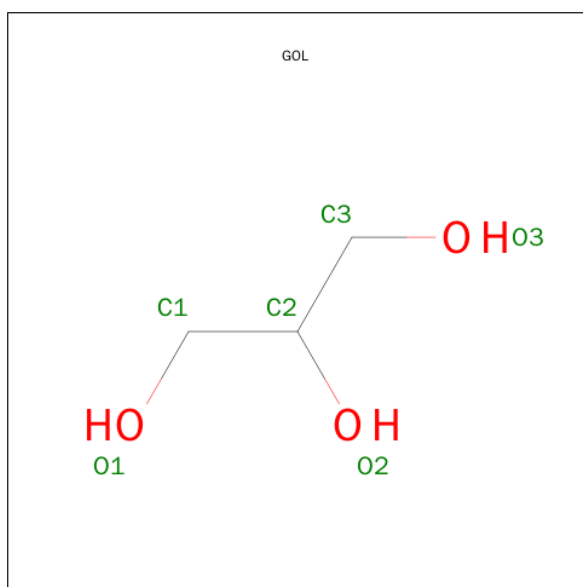
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			2	2		
3	C	1	Total	O	0	0
			2	2		
3	D	1	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			2	2		
3	F	1	Total	O	0	0
			2	2		

- Molecule 4 is FORMYL GROUP (three-letter code: FOR) (formula: CH<sub>2</sub>O).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

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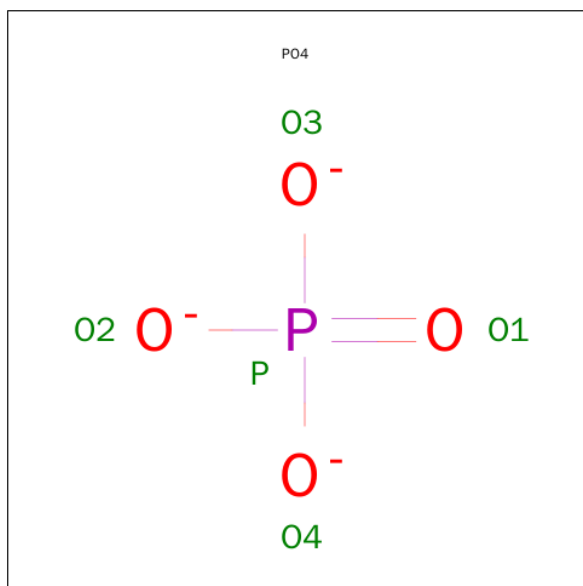
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	757	Total	O	0	0
			757	757		
7	B	734	Total	O	0	0
			734	734		
7	C	727	Total	O	0	0
			727	727		
7	D	732	Total	O	0	0
			732	732		
7	E	726	Total	O	0	0
			726	726		
7	F	709	Total	O	0	0
			709	709		



V672
HIS
LYS
GLU
THR
LYS
THR
ASP
LYS
THR
ARG
ARG
LEU
ALA
PHE
GLU
GLY
SER
CYS
CYS
GLY
LYS

- Molecule 1: Peroxisomal primary amine oxidase

Chain D: 86% 8% 5%

MET	GLU	ARG	LEU	ARG	GLN	ILE	ALA	SER	GLN	ALA	THR	ALA	ALA	SER	ALA	A17	P21	K34	K41	B57	K68	R77	L109	V118	E119	D120	L121	C122	S123	T124	E147	K150	P155	R169	V175	L190	R202	R211	R212	R213	R217
N222	E227	R236	Y272	G275	M328	T329	K339	T342	H343	R352	D355	H366	D369	V388	Q398	A403	H404	Y405	E406	Y407	M414	R420	L425	R467	D471	E501	M514	R521	H568	Y575	K576	R579	L580								
M601	F631	P632	L633	M634	P635	V672	HIS	LYS	GLU	THR	LYS	ASP	THR	ARG	LEU	ALA	PHE	GLU	GLY	SER	CYS	CYS	GLY	LYS																	

- Molecule 1: Peroxisomal primary amine oxidase

Chain E: 85% 10% 5%

W565	A566	S567	R579	L580	T581	P582	D604	D610	F631	P632	L633	M634	P635	V672	HIS	LYS	GLU	THR	LYS	ASP	LYS	THR	SER	ARG	LEU	ALA	PHE	GLY	GLY	SER	CYS	CYS	GLY	LYS				
G275	M301	I302	V303	L318	D319	M328	T329	N330	C338	K339	G340	V341	I342	H343	Y344	H348	D351	D355	K360	N361	H366	N382	S397	Q398	A402	N404	Y405	E406	Y407	R420	L425	M430	E439	A440	G441	Q457	D469	R521
GLU	ARG	LEU	ARG	GLN	ILE	ALA	SER	GLN	ALA	ALA	SER	ALA	ALA	SER	A17	R20	P21	K34	A45	K48	K68	R77	L84	L109	V118	E119	D120	C122	V175	L190	R213	N222	E227	E230	R236	Q246	P259	R265

- Molecule 1: Peroxisomal primary amine oxidase

Chain F: 88% 7% 5%

GLU	GLY	SER	CYS	GLY	LYS	K375	N382	V388	T389	R390	S397	Q398	A402	A403	H404	Y405	M414	Q415	D416	R420	L425	Q457	S461	R467	R521	W565	F631	P632	L633	M634	P635	R644	Y661	R670	V672	HIS	LYS	GLU	THR	LYS	ASP	LYS	THR	SER	ARG	LEU	ALA	PHE
MET	GLU	ARG	LEU	ARG	GLN	ILE	ALA	SER	GLN	ALA	THR	ALA	ALA	SER	ALA	A17	Q66	L84	T106	V118	E119	D120	L121	C122	E126	P155	Q171	N222	H227	T245	G275	V303	M328	T329	L334	G335	D336	D337	R352	D355	C364							

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.58Å 222.84Å 103.62Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	49.03 – 2.10 49.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.03-2.10) 98.5 (49.01-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.129 , 0.180 0.140 , 0.187	Depositor DCC
$R_{free}$ test set	13480 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.1	EDS
Estimated twinning fraction	0.479 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 265725 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	36172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, FOR, PO4, PEO, 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	0.94	2/5384 (0.0%)	0.94	10/7327 (0.1%)
1	B	0.95	1/5371 (0.0%)	0.96	17/7310 (0.2%)
1	C	0.92	2/5406 (0.0%)	0.95	10/7358 (0.1%)
1	D	0.94	1/5395 (0.0%)	0.95	10/7343 (0.1%)
1	E	0.91	2/5367 (0.0%)	0.97	16/7305 (0.2%)
1	F	0.94	2/5383 (0.0%)	0.91	6/7326 (0.1%)
All	All	0.93	10/32306 (0.0%)	0.95	69/43969 (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	A	0	1
1	C	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	126	GLU	CG-CD	6.39	1.61	1.51
1	E	567	SER	CB-OG	-6.37	1.33	1.42
1	C	126	GLU	CG-CD	5.65	1.60	1.51
1	E	230	GLU	CG-CD	5.45	1.60	1.51
1	C	122	CYS	CB-SG	5.41	1.91	1.82

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	610	ASP	CB-CG-OD1	8.35	125.81	118.30
1	E	213	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	352	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	B	644	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	E	521	ARG	NE-CZ-NH2	-7.82	116.39	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	LEU	Peptide
1	C	333	SER	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	5249	0	5079	66	0
1	B	5230	0	5072	46	1
1	C	5253	0	5110	58	0
1	D	5245	0	5089	48	0
1	E	5223	0	5071	43	0
1	F	5236	0	5085	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	D	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	78	0	104	5	0
5	B	54	0	71	2	0
5	C	42	0	56	2	0
5	D	54	0	72	9	0
5	E	30	0	40	3	0
5	F	54	0	72	1	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	F	5	0	0	0	0
7	A	757	0	0	14	1
7	B	734	0	0	15	0
7	C	727	0	0	27	0
7	D	732	0	0	22	0
7	E	726	0	0	21	1
7	F	709	0	0	20	1
All	All	36172	0	30921	300	2

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 5.

The worst 5 of 300 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:F:328[B]:MET:HE2	7:F:1554:HOH:O	1.06	1.22
1:E:118:VAL:O	7:E:1311:HOH:O	1.72	1.06
1:A:15:SER:CB	1:A:16:ALA:HB2	1.87	1.04
1:D:120:ASP:OD2	7:D:1367:HOH:O	1.74	1.04
1:A:15:SER:CB	1:A:35:ALA:HB2	1.89	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:CB	7:F:1242:HOH:O[2_655]	1.90	0.30
7:A:1492:HOH:O	7:E:1570:HOH:O[1_655]	2.15	0.05

## 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	660/692 (95%)	635 (96%)	22 (3%)	3 (0%)	34	30
1	B	659/692 (95%)	637 (97%)	20 (3%)	2 (0%)	46	45
1	C	663/692 (96%)	633 (96%)	25 (4%)	5 (1%)	24	17
1	D	662/692 (96%)	638 (96%)	22 (3%)	2 (0%)	46	45
1	E	658/692 (95%)	637 (97%)	20 (3%)	1 (0%)	52	53
1	F	660/692 (95%)	634 (96%)	23 (4%)	3 (0%)	34	30
All	All	3962/4152 (95%)	3814 (96%)	132 (3%)	16 (0%)	39	37

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	C	333	SER
1	C	334	LEU
1	C	336	CYS
1	F	334	LEU

### 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	570/593 (96%)	561 (98%)	9 (2%)	70	76
1	B	570/593 (96%)	558 (98%)	12 (2%)	61	66
1	C	575/593 (97%)	571 (99%)	4 (1%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	574/593 (97%)	565 (98%)	9 (2%)	70	76
1	E	570/593 (96%)	560 (98%)	10 (2%)	66	72
1	F	572/593 (96%)	569 (100%)	3 (0%)	92	95
All	All	3431/3558 (96%)	3384 (99%)	47 (1%)	76	80

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	76	PRO
1	D	109	LEU
1	E	397[B]	SER
1	C	329	THR
1	D	202	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	66	GLN
1	C	330	ASN
1	F	330	ASN
1	C	70	GLN
1	C	218	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1	12,14,15	1.86	3 (25%)	10,19,21	2.29	3 (30%)
1	TYY	B	405	1	12,14,15	1.90	4 (33%)	10,19,21	2.23	3 (30%)
1	TYY	C	405	1	12,14,15	1.71	2 (16%)	10,19,21	2.22	4 (40%)
1	TYY	D	405	1	12,14,15	1.63	4 (33%)	10,19,21	2.66	4 (40%)
1	TYY	E	405	1	12,14,15	1.56	3 (25%)	10,19,21	2.17	5 (50%)
1	TYY	F	405	1	12,14,15	1.59	3 (25%)	10,19,21	1.76	4 (40%)

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	1	-	0/4/22/24	0/1/1/1
1	TYY	B	405	1	-	0/4/22/24	0/1/1/1
1	TYY	C	405	1	-	0/4/22/24	0/1/1/1
1	TYY	D	405	1	-	0/4/22/24	0/1/1/1
1	TYY	E	405	1	-	0/4/22/24	0/1/1/1
1	TYY	F	405	1	-	0/4/22/24	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405	TYY	CG-CD1	-3.36	1.44	1.49
1	A	405	TYY	CD2-CE2	-2.69	1.37	1.42
1	F	405	TYY	CE1-CD1	-2.49	1.37	1.44
1	D	405	TYY	CG-CD1	-2.16	1.46	1.49
1	E	405	TYY	CE1-CD1	-2.14	1.38	1.44

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	TYY	OZ-CD1-CG	-6.73	114.98	120.85
1	A	405	TYY	OZ-CD1-CG	-5.33	116.20	120.85
1	B	405	TYY	OZ-CD1-CG	-5.30	116.22	120.85
1	C	405	TYY	OZ-CD1-CG	-4.08	117.29	120.85
1	C	405	TYY	CE1-CZ-CE2	-3.21	117.61	121.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	TYY	1	0
1	C	405	TYY	4	0
1	D	405	TYY	3	0
1	E	405	TYY	2	0
1	F	405	TYY	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 6 are monoatomic - leaving 64 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	PEO	A	802	2	1,1,1	1.89	0	0,0,0	0.00	-
4	FOR	A	803	-	0,1,1	0.00	-	0,0,0	0.00	-
5	GOL	A	804	-	5,5,5	0.69	0	5,5,5	0.92	0
5	GOL	A	805	-	5,5,5	0.76	0	5,5,5	1.03	0
5	GOL	A	806	-	5,5,5	0.51	0	5,5,5	1.12	1 (20%)
5	GOL	A	807	-	5,5,5	0.42	0	5,5,5	0.90	0
5	GOL	A	808	-	5,5,5	0.40	0	5,5,5	1.03	0
5	GOL	A	809	-	5,5,5	0.80	0	5,5,5	0.66	0
5	GOL	A	810	-	5,5,5	0.38	0	5,5,5	0.89	0
5	GOL	A	811	-	5,5,5	0.48	0	5,5,5	0.44	0
5	GOL	A	812	-	5,5,5	0.32	0	5,5,5	0.32	0
5	GOL	A	813	-	5,5,5	0.63	0	5,5,5	0.98	0
5	GOL	A	814	-	5,5,5	0.56	0	5,5,5	0.61	0
5	GOL	A	815	-	5,5,5	0.32	0	5,5,5	0.72	0
5	GOL	A	816	-	5,5,5	0.43	0	5,5,5	0.49	0
3	PEO	B	802	2	1,1,1	1.72	0	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FOR	B	803	-	0,1,1	0.00	-	0,0,0	0.00	-
5	GOL	B	804	-	5,5,5	0.34	0	5,5,5	0.80	0
5	GOL	B	805	-	5,5,5	0.64	0	5,5,5	1.48	2 (40%)
5	GOL	B	806	-	5,5,5	0.44	0	5,5,5	0.41	0
5	GOL	B	807	-	5,5,5	0.26	0	5,5,5	0.62	0
5	GOL	B	808	-	5,5,5	0.69	0	5,5,5	0.66	0
5	GOL	B	809	-	5,5,5	0.94	0	5,5,5	0.62	0
5	GOL	B	810	-	5,5,5	0.38	0	5,5,5	1.12	0
5	GOL	B	811	-	5,5,5	0.41	0	5,5,5	0.90	0
6	PO4	B	812	-	4,4,4	0.48	0	6,6,6	0.28	0
5	GOL	B	813	-	5,5,5	0.39	0	5,5,5	0.34	0
3	PEO	C	802	2	1,1,1	2.52	1 (100%)	0,0,0	0.00	-
5	GOL	C	803	-	5,5,5	0.29	0	5,5,5	0.58	0
5	GOL	C	804	-	5,5,5	0.86	0	5,5,5	0.62	0
5	GOL	C	805	-	5,5,5	0.61	0	5,5,5	0.88	0
5	GOL	C	806	-	5,5,5	0.25	0	5,5,5	0.78	0
5	GOL	C	807	-	5,5,5	0.34	0	5,5,5	0.96	0
6	PO4	C	808	-	4,4,4	0.39	0	6,6,6	0.29	0
5	GOL	C	809	-	5,5,5	0.72	0	5,5,5	0.35	0
5	GOL	C	810	-	5,5,5	0.53	0	5,5,5	0.65	0
3	PEO	D	701	2	1,1,1	2.30	1 (100%)	0,0,0	0.00	-
4	FOR	D	702	-	0,1,1	0.00	-	0,0,0	0.00	-
5	GOL	D	704	-	5,5,5	0.38	0	5,5,5	0.85	0
5	GOL	D	705	-	5,5,5	0.36	0	5,5,5	0.18	0
5	GOL	D	706	-	5,5,5	0.43	0	5,5,5	0.75	0
5	GOL	D	707	-	5,5,5	0.41	0	5,5,5	1.09	0
5	GOL	D	708	-	5,5,5	0.26	0	5,5,5	1.35	1 (20%)
5	GOL	D	709	-	5,5,5	0.22	0	5,5,5	0.63	0
5	GOL	D	710	-	5,5,5	0.23	0	5,5,5	0.19	0
5	GOL	D	711	-	5,5,5	0.68	0	5,5,5	0.79	0
5	GOL	D	712	-	5,5,5	0.92	0	5,5,5	0.99	0
3	PEO	E	802	2	1,1,1	1.74	0	0,0,0	0.00	-
5	GOL	E	803	-	5,5,5	0.34	0	5,5,5	0.96	0
5	GOL	E	804	-	5,5,5	0.70	0	5,5,5	0.64	0
5	GOL	E	805	-	5,5,5	0.43	0	5,5,5	0.26	0
5	GOL	E	806	-	5,5,5	0.17	0	5,5,5	1.28	0
5	GOL	E	807	-	5,5,5	0.36	0	5,5,5	0.95	0
3	PEO	F	802	2	1,1,1	2.29	1 (100%)	0,0,0	0.00	-
5	GOL	F	803	-	5,5,5	0.54	0	5,5,5	0.67	0
5	GOL	F	804	-	5,5,5	0.45	0	5,5,5	1.41	1 (20%)
5	GOL	F	805	-	5,5,5	0.28	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	F	806	-	5,5,5	0.54	0	5,5,5	1.43	1 (20%)
5	GOL	F	807	-	5,5,5	0.57	0	5,5,5	0.80	0
5	GOL	F	808	-	5,5,5	0.32	0	5,5,5	0.57	0
6	PO4	F	809	-	4,4,4	0.25	0	6,6,6	0.28	0
5	GOL	F	810	-	5,5,5	0.24	0	5,5,5	0.52	0
5	GOL	F	811	-	5,5,5	0.83	0	5,5,5	0.60	0
5	GOL	F	812	-	5,5,5	0.71	0	5,5,5	0.90	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
3	PEO	A	802	2	-	0/0/0/0	0/0/0/0
4	FOR	A	803	-	-	0/0/0/0	0/0/0/0
5	GOL	A	804	-	-	0/4/4/4	0/0/0/0
5	GOL	A	805	-	-	0/4/4/4	0/0/0/0
5	GOL	A	806	-	-	0/4/4/4	0/0/0/0
5	GOL	A	807	-	-	0/4/4/4	0/0/0/0
5	GOL	A	808	-	-	0/4/4/4	0/0/0/0
5	GOL	A	809	-	-	0/4/4/4	0/0/0/0
5	GOL	A	810	-	-	0/4/4/4	0/0/0/0
5	GOL	A	811	-	-	0/4/4/4	0/0/0/0
5	GOL	A	812	-	-	0/4/4/4	0/0/0/0
5	GOL	A	813	-	-	0/4/4/4	0/0/0/0
5	GOL	A	814	-	-	0/4/4/4	0/0/0/0
5	GOL	A	815	-	-	0/4/4/4	0/0/0/0
5	GOL	A	816	-	-	0/4/4/4	0/0/0/0
3	PEO	B	802	2	-	0/0/0/0	0/0/0/0
4	FOR	B	803	-	-	0/0/0/0	0/0/0/0
5	GOL	B	804	-	-	0/4/4/4	0/0/0/0
5	GOL	B	805	-	-	0/4/4/4	0/0/0/0
5	GOL	B	806	-	-	0/4/4/4	0/0/0/0
5	GOL	B	807	-	-	0/4/4/4	0/0/0/0
5	GOL	B	808	-	-	0/4/4/4	0/0/0/0
5	GOL	B	809	-	-	0/4/4/4	0/0/0/0
5	GOL	B	810	-	-	0/4/4/4	0/0/0/0
5	GOL	B	811	-	-	0/4/4/4	0/0/0/0
6	PO4	B	812	-	-	0/0/0/0	0/0/0/0
5	GOL	B	813	-	-	0/4/4/4	0/0/0/0
3	PEO	C	802	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	803	-	-	0/4/4/4	0/0/0/0
5	GOL	C	804	-	-	0/4/4/4	0/0/0/0
5	GOL	C	805	-	-	0/4/4/4	0/0/0/0
5	GOL	C	806	-	-	0/4/4/4	0/0/0/0
5	GOL	C	807	-	-	0/4/4/4	0/0/0/0
6	PO4	C	808	-	-	0/0/0/0	0/0/0/0
5	GOL	C	809	-	-	0/4/4/4	0/0/0/0
5	GOL	C	810	-	-	0/4/4/4	0/0/0/0
3	PEO	D	701	2	-	0/0/0/0	0/0/0/0
4	FOR	D	702	-	-	0/0/0/0	0/0/0/0
5	GOL	D	704	-	-	0/4/4/4	0/0/0/0
5	GOL	D	705	-	-	0/4/4/4	0/0/0/0
5	GOL	D	706	-	-	0/4/4/4	0/0/0/0
5	GOL	D	707	-	-	0/4/4/4	0/0/0/0
5	GOL	D	708	-	-	0/4/4/4	0/0/0/0
5	GOL	D	709	-	-	0/4/4/4	0/0/0/0
5	GOL	D	710	-	-	0/4/4/4	0/0/0/0
5	GOL	D	711	-	-	0/4/4/4	0/0/0/0
5	GOL	D	712	-	-	0/4/4/4	0/0/0/0
3	PEO	E	802	2	-	0/0/0/0	0/0/0/0
5	GOL	E	803	-	-	0/4/4/4	0/0/0/0
5	GOL	E	804	-	-	0/4/4/4	0/0/0/0
5	GOL	E	805	-	-	0/4/4/4	0/0/0/0
5	GOL	E	806	-	-	0/4/4/4	0/0/0/0
5	GOL	E	807	-	-	0/4/4/4	0/0/0/0
3	PEO	F	802	2	-	0/0/0/0	0/0/0/0
5	GOL	F	803	-	-	0/4/4/4	0/0/0/0
5	GOL	F	804	-	-	0/4/4/4	0/0/0/0
5	GOL	F	805	-	-	0/4/4/4	0/0/0/0
5	GOL	F	806	-	-	0/4/4/4	0/0/0/0
5	GOL	F	807	-	-	0/4/4/4	0/0/0/0
5	GOL	F	808	-	-	0/4/4/4	0/0/0/0
6	PO4	F	809	-	-	0/0/0/0	0/0/0/0
5	GOL	F	810	-	-	0/4/4/4	0/0/0/0
5	GOL	F	811	-	-	0/4/4/4	0/0/0/0
5	GOL	F	812	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	PEO	O2-O1	-2.52	1.24	1.43
3	D	701	PEO	O2-O1	-2.30	1.26	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	PEO	O2-O1	-2.29	1.26	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	708	GOL	O1-C1-C2	-2.76	96.81	110.18
5	F	804	GOL	O3-C3-C2	-2.75	96.83	110.18
5	A	806	GOL	O3-C3-C2	-2.25	99.26	110.18
5	B	805	GOL	O2-C2-C1	-2.10	99.00	108.65
5	F	806	GOL	O2-C2-C1	-2.05	99.27	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	FOR	1	0
5	A	804	GOL	1	0
5	A	805	GOL	1	0
5	A	813	GOL	2	0
5	A	816	GOL	1	0
5	B	805	GOL	2	0
5	C	810	GOL	2	0
4	D	702	FOR	1	0
5	D	704	GOL	1	0
5	D	705	GOL	1	0
5	D	711	GOL	5	0
5	D	712	GOL	2	0
5	E	805	GOL	3	0
5	F	812	GOL	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, 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	657/692 (94%)	-0.81	2 (0%) 94 95	12, 19, 36, 77	0
1	B	657/692 (94%)	-0.80	4 (0%) 90 92	12, 19, 35, 84	0
1	C	655/692 (94%)	-0.79	1 (0%) 95 96	12, 19, 41, 75	0
1	D	655/692 (94%)	-0.80	1 (0%) 95 96	13, 20, 38, 86	0
1	E	655/692 (94%)	-0.81	2 (0%) 94 95	13, 20, 38, 87	0
1	F	655/692 (94%)	-0.80	1 (0%) 95 96	12, 19, 40, 75	0
All	All	3934/4152 (94%)	-0.80	11 (0%) 94 95	12, 19, 38, 87	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	672	VAL	4.7
1	D	672	VAL	4.3
1	A	16	ALA	4.2
1	B	16	ALA	4.0
1	B	334	LEU	3.7

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TYY	F	405	14/15	0.97	0.09	-	14,25,41,46	0
1	TYY	A	405	14/15	0.97	0.09	-	14,21,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TYY	D	405	14/15	0.97	0.09	-	16,24,40,50	0
1	TYY	B	405	14/15	0.97	0.08	-	16,23,35,41	0
1	TYY	C	405	14/15	0.95	0.11	-	16,23,44,46	0
1	TYY	E	405	14/15	0.97	0.09	-	16,23,36,41	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FOR	B	803	2/2	0.90	0.31	35.60	56,56,56,56	2
4	FOR	D	702	2/2	0.81	0.31	30.96	57,57,57,62	0
4	FOR	A	803	2/2	0.91	0.27	22.05	68,68,68,70	0
5	GOL	E	804	6/6	0.84	0.19	14.85	43,55,59,59	0
5	GOL	F	810	6/6	0.88	0.29	13.98	54,74,77,78	0
5	GOL	A	807	6/6	0.94	0.16	12.50	46,49,50,51	0
5	GOL	D	706	6/6	0.91	0.16	12.26	53,55,59,60	0
5	GOL	A	815	6/6	0.93	0.16	11.72	41,55,58,61	0
5	GOL	C	807	6/6	0.92	0.13	11.14	46,50,53,56	0
5	GOL	A	809	6/6	0.97	0.18	10.86	23,28,29,30	0
5	GOL	F	806	6/6	0.92	0.16	10.51	50,54,56,59	0
5	GOL	F	807	6/6	0.96	0.14	10.48	36,41,47,48	0
5	GOL	B	806	6/6	0.92	0.14	9.92	46,49,50,53	0
5	GOL	A	814	6/6	0.94	0.16	9.89	47,50,52,53	0
5	GOL	F	811	6/6	0.95	0.17	8.56	24,27,29,30	0
5	GOL	C	810	6/6	0.94	0.16	8.05	41,55,57,62	0
5	GOL	B	809	6/6	0.94	0.17	7.70	23,30,31,31	0
5	GOL	F	808	6/6	0.95	0.13	7.63	50,52,53,59	0
5	GOL	A	810	6/6	0.85	0.18	7.57	45,53,55,56	0
5	GOL	E	806	6/6	0.91	0.18	6.95	39,40,43,43	0
5	GOL	B	810	6/6	0.85	0.20	6.82	43,57,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	808	6/6	0.96	0.16	6.39	23,24,27,28	0
5	GOL	C	803	6/6	0.96	0.16	6.26	28,37,39,41	0
5	GOL	A	816	6/6	0.92	0.15	5.94	53,60,61,63	0
5	GOL	D	711	6/6	0.78	0.16	5.76	46,60,62,68	0
5	GOL	D	712	6/6	0.86	0.17	5.27	35,48,49,51	0
5	GOL	D	704	6/6	0.96	0.12	5.11	44,49,53,56	0
5	GOL	E	805	6/6	0.95	0.15	5.00	44,47,57,60	0
5	GOL	F	803	6/6	0.96	0.15	4.84	30,34,38,39	0
5	GOL	D	709	6/6	0.94	0.17	4.66	35,41,44,52	0
3	PEO	F	802	2/2	0.98	0.14	4.13	13,13,13,16	0
3	PEO	C	802	2/2	0.98	0.14	3.95	14,14,14,17	0
5	GOL	F	805	6/6	0.91	0.14	3.90	52,61,67,72	0
5	GOL	A	813	6/6	0.91	0.14	3.56	40,45,47,49	0
5	GOL	A	804	6/6	0.98	0.10	3.43	22,32,33,40	0
5	GOL	B	805	6/6	0.91	0.13	3.17	35,52,59,60	0
5	GOL	F	804	6/6	0.94	0.13	3.14	39,42,44,47	0
5	GOL	C	806	6/6	0.90	0.14	2.95	36,44,45,47	0
3	PEO	B	802	2/2	0.99	0.11	2.57	13,13,13,21	0
5	GOL	F	812	6/6	0.90	0.14	2.53	42,44,47,54	0
3	PEO	E	802	2/2	0.99	0.11	2.50	14,14,14,20	0
5	GOL	B	811	6/6	0.94	0.14	2.45	46,48,56,57	0
5	GOL	C	809	6/6	0.97	0.10	2.42	24,31,33,40	0
5	GOL	E	807	6/6	0.98	0.14	2.30	33,35,38,38	0
5	GOL	C	804	6/6	0.90	0.12	2.02	39,42,46,50	0
3	PEO	D	701	2/2	0.98	0.10	1.67	17,17,17,17	0
5	GOL	B	813	6/6	0.96	0.11	1.23	43,45,46,54	0
5	GOL	D	707	6/6	0.95	0.12	1.18	29,36,41,41	0
2	CU	A	801	1/1	1.00	0.09	1.02	19,19,19,19	0
3	PEO	A	802	2/2	0.99	0.09	0.98	14,14,14,20	0
5	GOL	B	804	6/6	0.92	0.09	0.95	38,40,43,46	0
5	GOL	A	812	6/6	0.96	0.11	0.81	45,46,48,54	0
5	GOL	A	805	6/6	0.92	0.11	0.71	40,45,49,51	0
5	GOL	A	806	6/6	0.95	0.09	0.46	34,38,42,45	0
5	GOL	D	708	6/6	0.97	0.10	0.45	35,37,40,40	0
5	GOL	E	803	6/6	0.97	0.09	0.32	41,48,56,58	0
2	CU	E	801	1/1	1.00	0.08	-0.06	20,20,20,20	0
2	CU	F	801	1/1	1.00	0.07	-	19,19,19,19	0
5	GOL	B	807	6/6	0.94	0.10	-	42,51,55,56	1
5	GOL	D	710	6/6	0.87	0.26	-	62,64,69,77	0
5	GOL	A	811	6/6	0.94	0.11	-	44,45,46,52	0
6	PO4	B	812	5/5	0.95	0.12	-	31,33,34,35	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	B	801	1/1	1.00	0.09	-	20,20,20,20	0
5	GOL	D	705	6/6	0.45	0.43	-	89,99,102,117	0
2	CU	C	801	1/1	1.00	0.07	-	19,19,19,19	0
2	CU	D	703	1/1	1.00	0.08	-	20,20,20,20	0
5	GOL	A	808	6/6	0.91	0.13	-	52,57,58,60	0
6	PO4	F	809	5/5	0.96	0.09	-	44,52,59,62	0
6	PO4	C	808	5/5	0.97	0.10	-	43,49,60,61	0
5	GOL	C	805	6/6	0.96	0.12	-	47,48,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.