



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:06 am BST

PDB ID : 4KFD
Title : Crystal structure of Hansenula polymorpha copper amine oxidase-1 reduced by methylamine at pH 6.0
Authors : Johnson, B.J.; Yukl, E.T.; Klema, V.J.; Wilmot, C.M.
Deposited on : 2013-04-26
Resolution : 1.69 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 ⓘ symbol.

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

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

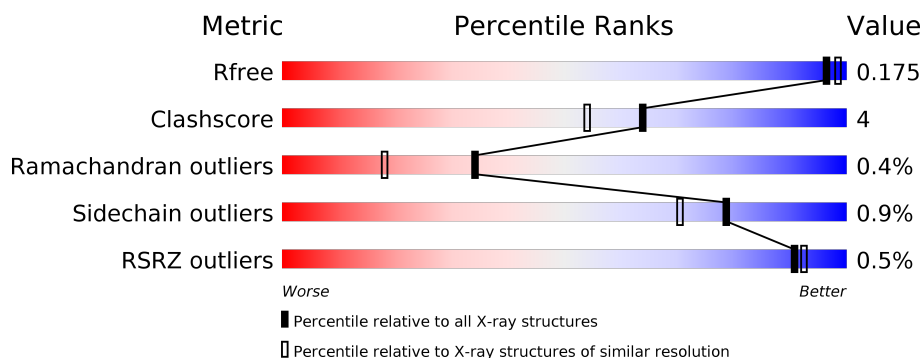
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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>86%</div> <div>8% • 5%</div> </div>
1	B	692	<div> <div>87%</div> <div>7% 5%</div> </div>
1	C	692	<div> <div>85%</div> <div>8% • 5%</div> </div>
1	D	692	<div> <div>86%</div> <div>8% • 5%</div> </div>
1	E	692	<div> <div>86%</div> <div>8% • 5%</div> </div>
1	F	692	<div> <div>87%</div> <div>7% • 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TYY	C	405[A]	-	-	X	-
1	TYY	F	405[A]	-	-	X	-
3	PEO	A	802	-	X	-	-
3	PEO	B	802	-	X	-	-
3	PEO	C	802	-	X	-	-
3	PEO	D	802	-	X	-	-
3	PEO	E	802	-	X	-	-
3	PEO	F	802	-	X	-	-
4	GOL	D	804	-	-	-	X
4	GOL	D	808	-	-	X	-
4	GOL	D	811	-	-	X	-
4	GOL	E	807	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36394 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.

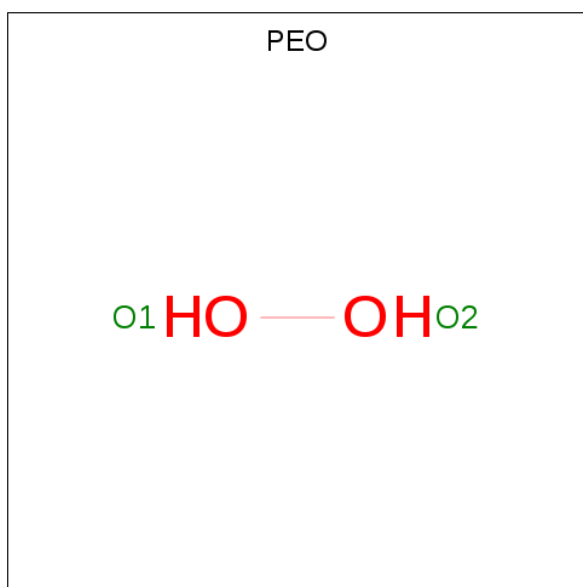
- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	5	0
			5239	3332	902	981	24			
1	B	656	Total	C	N	O	S	0	5	0
			5224	3325	896	979	24			
1	C	655	Total	C	N	O	S	0	11	0
			5262	3353	901	983	25			
1	D	655	Total	C	N	O	S	0	8	0
			5232	3331	897	980	24			
1	E	655	Total	C	N	O	S	0	5	0
			5218	3323	895	976	24			
1	F	656	Total	C	N	O	S	0	8	0
			5250	3343	900	982	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: H₂O₂).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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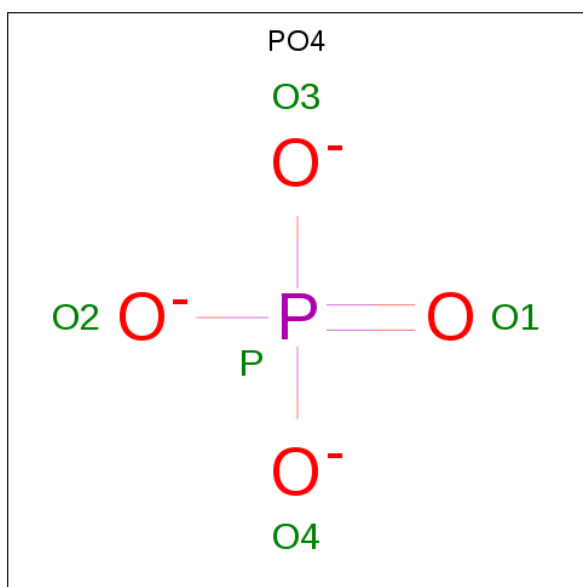
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total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

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

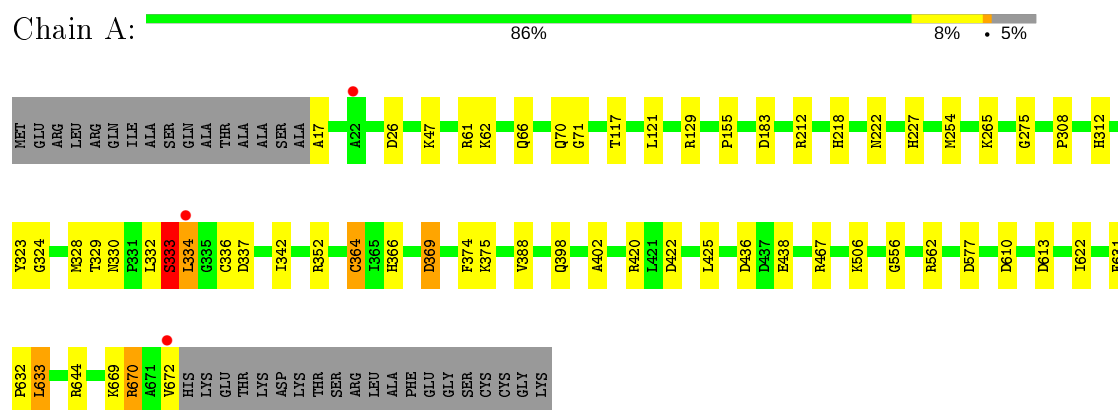
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	809	Total	O	0	0
			809	809		
6	B	771	Total	O	0	0
			771	771		
6	C	765	Total	O	0	0
			765	765		
6	D	774	Total	O	0	0
			774	774		
6	E	760	Total	O	0	0
			760	760		
6	F	745	Total	O	0	0
			745	745		

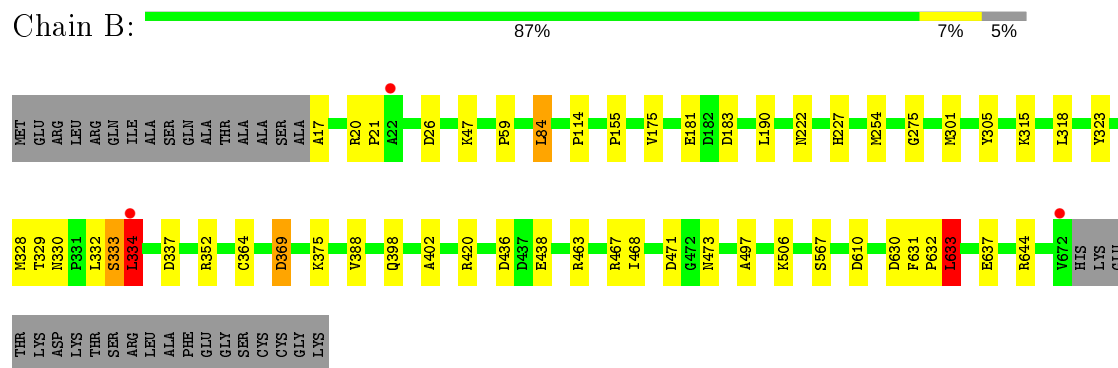
3 Residue-property plots [i](#)

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.

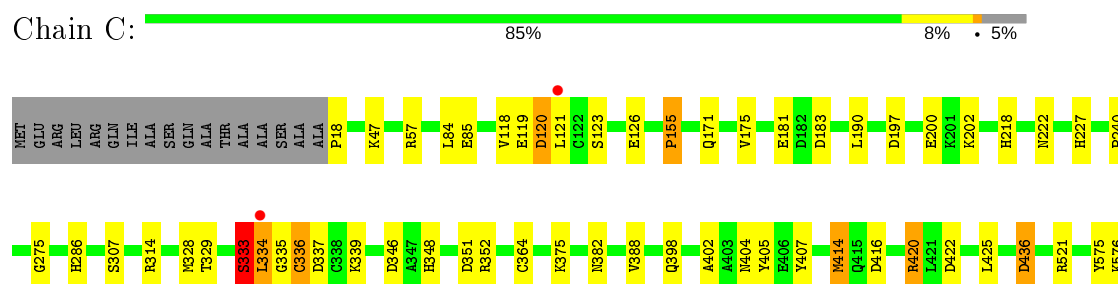
- Molecule 1: Peroxisomal primary amine oxidase

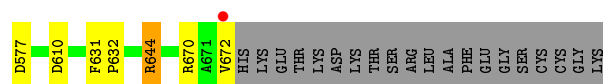


- Molecule 1: Peroxisomal primary amine oxidase



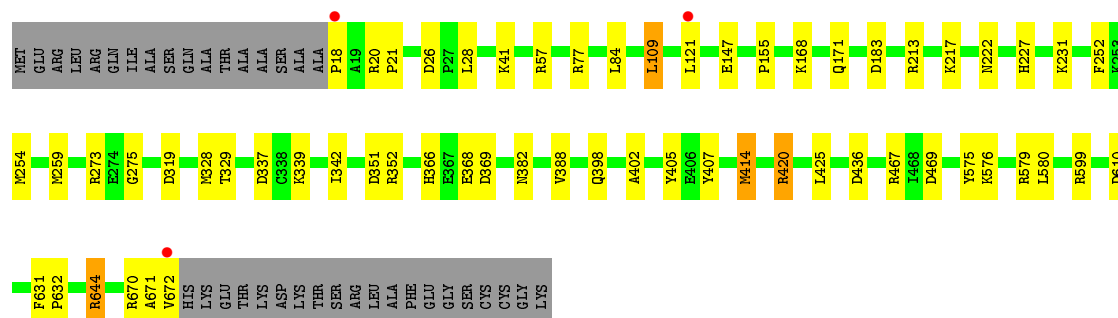
- Molecule 1: Peroxisomal primary amine oxidase





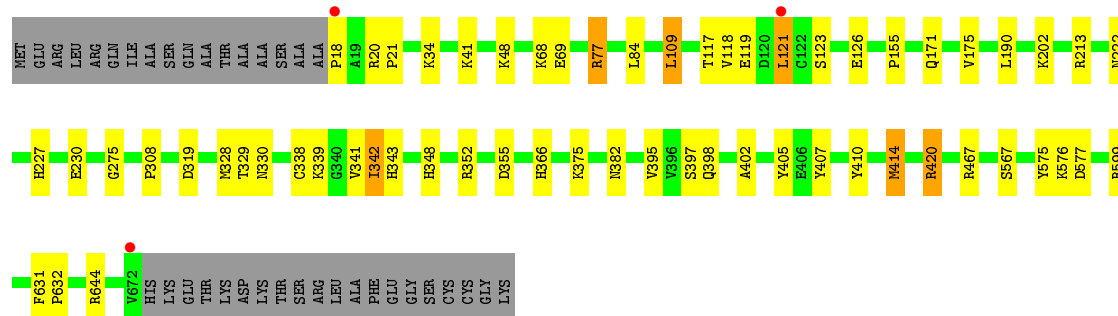
- Molecule 1: Peroxisomal primary amine oxidase

Chain D: 86% 8% 5%



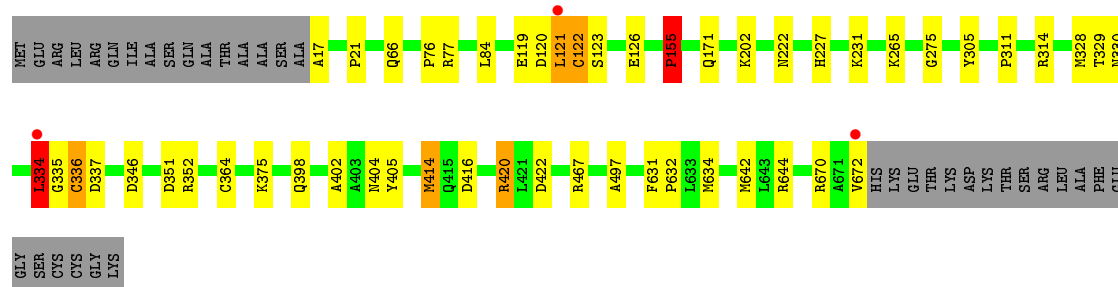
- Molecule 1: Peroxisomal primary amine oxidase

Chain E: 86% 8% 5%



- Molecule 1: Peroxisomal primary amine oxidase

Chain F: 87% 7% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.58Å 222.84Å 103.62Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	46.78 – 1.69 46.78 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.78-1.69) 99.4 (46.78-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.134 , 0.164 0.148 , 0.175	Depositor DCC
R_{free} test set	25742 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.480 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36394	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.99	4/5374 (0.1%)	1.02	20/7313 (0.3%)
1	B	0.99	6/5368 (0.1%)	1.03	17/7306 (0.2%)
1	C	1.01	4/5401 (0.1%)	1.02	16/7350 (0.2%)
1	D	1.02	2/5382 (0.0%)	1.03	23/7324 (0.3%)
1	E	1.02	6/5362 (0.1%)	1.02	15/7297 (0.2%)
1	F	0.99	2/5383 (0.0%)	1.00	14/7326 (0.2%)
All	All	1.00	24/32270 (0.1%)	1.02	105/43916 (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	B	0	1
1	C	0	2
1	F	0	1
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	126	GLU	CG-CD	6.80	1.62	1.51
1	E	567	SER	CB-OG	-6.54	1.33	1.42
1	A	556	GLY	N-CA	-6.46	1.36	1.46
1	F	364	CYS	CB-SG	-6.44	1.71	1.82
1	E	230	GLU	CD-OE1	6.44	1.32	1.25
1	E	230	GLU	CG-CD	6.22	1.61	1.51
1	C	126	GLU	CG-CD	5.98	1.60	1.51
1	B	305	TYR	CE2-CZ	5.87	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	171	GLN	CD-NE2	-5.84	1.18	1.32
1	C	364	CYS	CB-SG	-5.71	1.72	1.81
1	E	171	GLN	CD-NE2	-5.61	1.18	1.32
1	A	71	GLY	N-CA	-5.60	1.37	1.46
1	B	637	GLU	CD-OE2	5.59	1.31	1.25
1	B	438	GLU	CD-OE2	5.59	1.31	1.25
1	E	230	GLU	CD-OE2	5.52	1.31	1.25
1	C	307	SER	CB-OG	5.34	1.49	1.42
1	C	181	GLU	CD-OE1	-5.24	1.19	1.25
1	A	438	GLU	CD-OE2	5.22	1.31	1.25
1	A	467	ARG	CB-CG	-5.22	1.38	1.52
1	B	364	CYS	CB-SG	-5.20	1.73	1.81
1	D	414	MET	SD-CE	-5.19	1.48	1.77
1	B	467	ARG	CB-CG	-5.17	1.38	1.52
1	B	567	SER	CB-OG	-5.14	1.35	1.42
1	E	407	TYR	CG-CD1	-5.12	1.32	1.39

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	NE-CZ-NH1	-11.26	114.67	120.30
1	A	352	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	B	352	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	D	352	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	B	254	MET	CG-SD-CE	-8.98	85.83	100.20
1	B	333	SER	N-CA-C	-8.45	88.19	111.00
1	E	420	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	352	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	254	MET	CG-SD-CE	-7.89	87.57	100.20
1	D	352	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	414	MET	CG-SD-CE	-7.80	87.72	100.20
1	E	599	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	644	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	C	644	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	644	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	C	120	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	B	420	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	C	420	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	467	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	D	644	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	E	414	MET	CG-SD-CE	-7.10	88.84	100.20
1	A	633	LEU	CB-CG-CD2	7.04	122.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	420	ARG	CA-CB-CG	6.96	128.71	113.40
1	F	351	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	577	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	C	422	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	633	LEU	CB-CG-CD2	6.73	122.44	111.00
1	D	168	LYS	CD-CE-NZ	-6.71	96.27	111.70
1	B	334	LEU	CA-CB-CG	6.71	130.73	115.30
1	E	352	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	D	579	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	610	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	109	LEU	CB-CG-CD1	6.66	122.32	111.00
1	E	644	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	F	346	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	212	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	D	599	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	613	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	351	ASP	CB-CG-OD1	6.36	124.02	118.30
1	C	436	ASP	CB-CG-OD1	6.35	124.01	118.30
1	F	121	LEU	CB-CA-C	-6.22	98.39	110.20
1	B	26	ASP	CB-CG-OD1	6.17	123.85	118.30
1	F	346	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	369[A]	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	369[B]	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	467	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	D	388	VAL	CB-CA-C	-6.09	99.83	111.40
1	D	414	MET	CG-SD-CE	-6.08	90.48	100.20
1	B	471	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	420	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	26	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	521	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	610	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	346	ASP	CB-CG-OD1	5.81	123.53	118.30
1	F	414	MET	CG-SD-CE	-5.77	90.96	100.20
1	D	20	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	E	77	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	562	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	254	MET	CA-CB-CG	5.70	122.99	113.30
1	C	183	ASP	CB-CG-OD1	5.65	123.39	118.30
1	F	420	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	F	644	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	183	ASP	CB-CG-OD1	5.60	123.34	118.30
1	E	467	ARG	NE-CZ-NH2	-5.59	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	337	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	630	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	E	77	ARG	CG-CD-NE	-5.55	100.14	111.80
1	C	610	ASP	CB-CG-OD1	5.51	123.26	118.30
1	E	342	ILE	CA-CB-CG2	5.51	121.92	110.90
1	A	183	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	D	351	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	E	20	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	436	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	129	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	F	314	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	E	420	ARG	CA-CB-CG	5.40	125.29	113.40
1	F	416	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	26	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	333	SER	N-CA-C	5.36	125.47	111.00
1	C	351	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	388	VAL	CB-CA-C	-5.35	101.23	111.40
1	D	436	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	183	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	463	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	633	LEU	CB-CG-CD1	5.32	120.05	111.00
1	C	197	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	F	351	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	E	109	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	670	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	334	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	84	LEU	CB-CG-CD1	5.25	119.93	111.00
1	C	416	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	28	LEU	CB-CG-CD2	5.24	119.90	111.00
1	D	273	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	E	121	LEU	CB-CG-CD2	5.17	119.78	111.00
1	A	422	ASP	CB-CG-OD1	5.15	122.94	118.30
1	D	610	ASP	CB-CG-OD1	5.15	122.94	118.30
1	F	422	ASP	CB-CG-OD1	5.11	122.90	118.30
1	E	123	SER	N-CA-CB	-5.09	102.86	110.50
1	D	420	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	577	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	E	577	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	346	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	C	314	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	469	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	LEU	Peptide
1	B	332	LEU	Peptide
1	C	155	PRO	Mainchain
1	C	333	SER	Peptide
1	F	155	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5239	0	5073	48	0
1	B	5224	0	5066	31	0
1	C	5262	0	5111	65	0
1	D	5232	0	5082	37	0
1	E	5218	0	5067	42	0
1	F	5250	0	5090	42	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	72	0	95	5	0
4	B	48	0	64	1	0
4	C	48	0	64	3	0
4	D	54	0	72	10	0
4	E	36	0	48	5	0
4	F	54	0	72	3	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	809	0	0	10	0
6	B	771	0	0	5	0
6	C	765	0	0	25	0
6	D	774	0	0	13	0
6	E	760	0	0	23	0
6	F	745	0	0	20	0
All	All	36394	0	30904	263	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 4.

All (263) 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	6:F:1589:HOH:O	1.18	1.30
1:F:405[A]:TYY:N5	6:F:1642:HOH:O	1.57	1.28
1:C:405[A]:TYY:CE2	6:C:1083:HOH:O	1.88	1.19
1:C:405[A]:TYY:N5	6:C:1660:HOH:O	1.76	1.16
1:F:328[B]:MET:CE	6:F:1589:HOH:O	1.72	1.15
1:F:405[A]:TYY:CE2	6:F:1169:HOH:O	1.97	1.11
1:D:328[B]:MET:HE2	6:D:1177:HOH:O	1.52	1.08
1:E:405:TYY:CE2	6:E:1248:HOH:O	2.02	1.07
1:D:405:TYY:CE2	6:D:1243:HOH:O	2.03	1.06
1:C:405[A]:TYY:CD2	6:C:1083:HOH:O	2.05	1.02
1:C:328[B]:MET:HE2	6:C:1540:HOH:O	1.60	1.01
1:C:328[B]:MET:CE	6:C:1540:HOH:O	2.06	1.01
1:C:334:LEU:HB3	1:C:335:GLY:HA2	1.49	0.95
4:E:805:GOL:H31	6:E:1524:HOH:O	1.65	0.94
1:B:17:ALA:N	6:B:1269:HOH:O	1.99	0.94
1:B:369[B]:ASP:OD2	6:B:1539:HOH:O	1.87	0.91
1:C:18:PRO:N	6:C:1294:HOH:O	2.04	0.91
1:D:328[B]:MET:CE	6:D:1177:HOH:O	2.07	0.91
1:A:17:ALA:N	6:A:1268:HOH:O	2.05	0.89
1:E:328[B]:MET:CE	6:E:1200:HOH:O	2.22	0.86
1:F:405[A]:TYY:CD2	6:F:1169:HOH:O	2.18	0.86
1:F:405[A]:TYY:N5	6:F:1248:HOH:O	1.72	0.85
1:B:468:ILE:H	1:B:473:ASN:HD21	1.25	0.84
1:D:57:ARG:HE	4:D:811:GOL:H2	1.42	0.84
1:D:18:PRO:N	4:D:808:GOL:HO1	1.76	0.84
1:A:369[A]:ASP:OD1	6:A:1703:HOH:O	1.96	0.82
1:C:414:MET:SD	1:C:420:ARG:NH1	2.53	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:GLY:HA3	1:C:336:CYS:HB2	1.63	0.81
1:C:121[B]:LEU:HD22	6:C:1634:HOH:O	1.82	0.79
1:E:405:TYY:CD2	6:E:1248:HOH:O	2.22	0.78
1:F:405[A]:TYY:OH	6:F:1248:HOH:O	1.90	0.78
1:C:405[A]:TYY:N5	6:C:1241:HOH:O	1.73	0.78
1:D:121:LEU:HB2	6:D:1646:HOH:O	1.82	0.77
1:E:18:PRO:N	6:E:1230:HOH:O	2.16	0.77
1:F:414:MET:SD	1:F:420:ARG:NH1	2.57	0.77
1:F:120:ASP:OD1	1:F:352:ARG:NH2	2.19	0.76
1:C:334:LEU:HB3	1:C:335:GLY:CA	2.14	0.75
1:A:436:ASP:H	4:A:804:GOL:H32	1.52	0.75
1:D:575:TYR:O	1:D:576:LYS:HD2	1.86	0.75
1:E:348:HIS:HD2	6:E:1225:HOH:O	1.68	0.75
1:E:328[B]:MET:HE3	6:E:1200:HOH:O	1.85	0.74
1:A:333:SER:HB2	6:A:1389:HOH:O	1.88	0.73
1:D:57:ARG:NE	4:D:811:GOL:H2	2.01	0.73
1:E:338:CYS:SG	1:E:342:ILE:HG12	2.29	0.73
1:E:328[B]:MET:HE2	6:E:1200:HOH:O	1.84	0.73
1:A:61:ARG:HH11	4:A:811:GOL:H11	1.53	0.72
1:C:328[B]:MET:HE3	6:C:1540:HOH:O	1.79	0.72
1:C:405[A]:TYY:OH	6:C:1241:HOH:O	1.95	0.72
1:D:319:ASP:OD2	6:D:1243:HOH:O	2.07	0.72
1:C:120:ASP:HB3	1:C:352:ARG:HH21	1.54	0.71
1:B:20:ARG:HB2	1:B:21:PRO:HD2	1.70	0.71
1:A:333:SER:HB3	1:A:334:LEU:C	2.11	0.71
1:E:414:MET:SD	1:E:420:ARG:NH1	2.64	0.70
1:E:575:TYR:O	1:E:576:LYS:HD2	1.91	0.70
1:E:41:LYS:HE3	6:E:944:HOH:O	1.92	0.69
1:D:405:TYY:CD2	6:D:1243:HOH:O	2.33	0.69
1:A:328[A]:MET:SD	1:A:402:ALA:HB2	2.33	0.68
1:F:405[A]:TYY:CZ	6:F:1248:HOH:O	2.35	0.68
1:A:117:THR:O	1:A:121[A]:LEU:HD13	1.95	0.67
1:A:333:SER:OG	1:A:336:CYS:HB2	1.95	0.67
1:C:118:VAL:HB	6:C:1500:HOH:O	1.95	0.67
1:C:339:LYS:NZ	6:C:1665:HOH:O	2.26	0.67
1:E:68:LYS:HE2	6:E:1653:HOH:O	1.96	0.66
1:B:328[A]:MET:SD	1:B:402:ALA:HB2	2.36	0.65
1:D:121:LEU:HD12	6:D:1646:HOH:O	1.95	0.65
1:A:333:SER:OG	1:A:337:ASP:N	2.27	0.64
1:D:57:ARG:HE	4:D:811:GOL:C2	2.08	0.64
1:C:333:SER:CB	1:C:335:GLY:HA3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:THR:O	1:E:121:LEU:HD23	1.98	0.64
1:A:333:SER:CB	1:A:336:CYS:H	2.10	0.64
1:C:382[A]:ASN:ND2	6:C:1286:HOH:O	2.31	0.64
1:F:405[A]:TYY:CE2	6:F:1248:HOH:O	2.27	0.64
1:C:348:HIS:HD2	6:C:1247:HOH:O	1.82	0.63
1:C:333:SER:HB2	1:C:335:GLY:HA3	1.80	0.63
1:A:669:LYS:HE3	1:B:181:GLU:OE1	1.99	0.63
1:F:122:CYS:N	6:F:1585:HOH:O	2.32	0.62
4:A:811:GOL:H32	6:A:1533:HOH:O	1.99	0.61
1:C:404:ASN:HD21	1:C:405[B]:TYY:CZ	2.13	0.61
1:A:62:LYS:NZ	1:A:66:GLN:HE22	1.99	0.61
1:A:333:SER:HB3	1:A:334:LEU:CA	2.31	0.60
1:D:414:MET:SD	1:D:420:ARG:NH1	2.73	0.60
1:C:335:GLY:CA	1:C:336:CYS:HB2	2.32	0.60
1:E:121:LEU:HB3	6:E:1659:HOH:O	2.02	0.60
1:C:575:TYR:O	1:C:576:LYS:HD2	2.02	0.59
1:F:404:ASN:HD21	1:F:405[B]:TYY:CZ	2.14	0.59
1:C:121[B]:LEU:HD21	6:C:1661:HOH:O	2.02	0.59
1:C:405[A]:TYY:CE2	6:C:1241:HOH:O	2.32	0.59
1:A:218:HIS:HE1	6:A:1257:HOH:O	1.86	0.59
1:A:506:LYS:HD2	6:A:1325:HOH:O	2.01	0.59
4:F:810:GOL:H2	6:F:1629:HOH:O	2.03	0.58
1:E:319:ASP:OD2	6:E:1248:HOH:O	2.17	0.58
1:E:338:CYS:SG	1:E:342:ILE:CG1	2.92	0.57
1:D:670:ARG:C	1:D:672:VAL:H	2.08	0.57
1:C:121[B]:LEU:CD2	6:C:1661:HOH:O	2.53	0.57
1:B:333:SER:CB	1:B:337:ASP:OD2	2.52	0.56
1:E:397[A]:SER:HG	1:E:410:TYR:HD1	1.53	0.56
1:B:333:SER:HB3	1:B:337:ASP:OD2	2.06	0.56
1:C:402:ALA:O	1:C:405[B]:TYY:HD2	2.05	0.56
1:F:402:ALA:O	1:F:405[B]:TYY:HD2	2.06	0.56
1:C:121[B]:LEU:HG	1:C:155:PRO:HG2	1.87	0.56
1:F:119:GLU:C	6:F:1585:HOH:O	2.44	0.55
1:D:18:PRO:CA	4:D:808:GOL:HO1	2.19	0.55
1:C:218:HIS:HE1	6:C:1126:HOH:O	1.90	0.54
1:C:18:PRO:N	6:C:1525:HOH:O	2.41	0.54
1:A:265:LYS:HE3	6:A:1356:HOH:O	2.06	0.54
1:C:333:SER:HB3	1:C:337:ASP:H	1.72	0.54
1:B:47:LYS:HE3	6:B:1361:HOH:O	2.07	0.54
1:B:315:LYS:NZ	6:B:1509:HOH:O	2.41	0.54
1:B:328[A]:MET:SD	1:B:402:ALA:CB	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:SER:CB	1:A:334:LEU:CA	2.86	0.53
1:B:275:GLY:HA3	1:B:398:GLN:HE22	1.73	0.53
1:F:642:MET:HE1	6:F:1541:HOH:O	2.09	0.53
1:A:328[A]:MET:SD	1:A:402:ALA:CB	2.96	0.53
1:A:275:GLY:HA3	1:A:398:GLN:HE22	1.73	0.53
1:A:323:TYR:HB2	1:A:328[A]:MET:HE2	1.91	0.53
1:E:202:LYS:NZ	6:E:1321:HOH:O	2.40	0.53
1:C:670:ARG:C	1:C:672:VAL:H	2.11	0.53
1:F:634:MET:SD	6:F:1444:HOH:O	2.59	0.53
1:A:62:LYS:HZ1	1:A:66:GLN:HE22	1.57	0.52
1:A:61:ARG:NH1	4:A:811:GOL:H11	2.22	0.52
1:B:631:PHE:CG	1:B:632:PRO:HA	2.43	0.52
1:E:275:GLY:HA3	1:E:398:GLN:HE22	1.75	0.52
4:E:804:GOL:H11	6:E:1656:HOH:O	2.10	0.52
1:C:333:SER:HB3	1:C:337:ASP:N	2.25	0.52
1:F:121:LEU:C	1:F:123:SER:H	2.12	0.52
1:D:275:GLY:HA3	1:D:398:GLN:HE22	1.76	0.51
1:E:330:ASN:HD22	1:F:375:LYS:NZ	2.08	0.51
1:C:57:ARG:NH2	4:C:810:GOL:O3	2.39	0.51
1:D:18:PRO:N	4:D:808:GOL:O1	2.40	0.51
1:F:670:ARG:NH2	6:F:1547:HOH:O	2.40	0.50
1:A:312:HIS:HD2	6:A:1271:HOH:O	1.93	0.50
1:D:382[A]:ASN:ND2	6:D:1211:HOH:O	2.44	0.50
1:C:670:ARG:HD2	6:C:1408:HOH:O	2.11	0.50
1:F:275:GLY:HA3	1:F:398:GLN:HE22	1.76	0.50
4:C:809:GOL:O2	1:D:231:LYS:HD3	2.10	0.50
1:A:631:PHE:CG	1:A:632:PRO:HA	2.47	0.49
1:D:407:TYR:CD1	1:D:425:LEU:CD2	2.95	0.49
1:E:330:ASN:HD22	1:F:375:LYS:HZ3	1.60	0.49
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.47	0.49
1:D:631:PHE:CG	1:D:632:PRO:HA	2.48	0.49
1:C:404:ASN:HD21	1:C:405[B]:TYY:CE1	2.26	0.49
1:D:18:PRO:N	4:D:808:GOL:H2	2.28	0.48
1:C:120:ASP:OD2	6:C:1400:HOH:O	2.20	0.48
1:F:17:ALA:N	6:F:1506:HOH:O	2.46	0.48
1:B:323:TYR:HB2	1:B:328[A]:MET:HE2	1.95	0.48
1:C:333:SER:HB2	1:C:335:GLY:CA	2.42	0.48
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.48	0.48
1:C:200:GLU:HB3	1:C:202:LYS:HE3	1.96	0.48
1:B:175[A]:VAL:HG11	1:B:190:LEU:HD12	1.95	0.47
1:A:333:SER:CB	1:A:334:LEU:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:GLY:HA3	1:C:398:GLN:HE22	1.79	0.47
1:E:341:VAL:C	1:E:342:ILE:HD12	2.35	0.47
1:E:68:LYS:HD2	6:E:1278:HOH:O	2.13	0.47
1:E:382:ASN:HB2	6:E:1561:HOH:O	2.14	0.47
1:F:335:GLY:O	1:F:337:ASP:N	2.48	0.47
1:A:121[A]:LEU:N	1:A:121[A]:LEU:CD1	2.78	0.47
1:B:333:SER:HB2	1:B:337:ASP:OD2	2.14	0.47
1:F:84:LEU:N	1:F:84:LEU:HD12	2.29	0.46
1:C:119:GLU:HB2	6:C:1109:HOH:O	2.14	0.46
1:D:407:TYR:CD1	1:D:425:LEU:HD22	2.50	0.46
1:B:468:ILE:N	1:B:473:ASN:HD21	2.04	0.46
1:F:222:ASN:HB3	1:F:227:HIS:CG	2.50	0.46
1:F:404:ASN:HD21	1:F:405[B]:TYY:CE1	2.29	0.46
1:D:369:ASP:OD1	6:D:1546:HOH:O	2.21	0.46
1:F:155:PRO:HB2	1:F:171:GLN:OE1	2.15	0.46
1:C:47:LYS:HG2	1:C:85:GLU:OE2	2.16	0.46
1:E:382:ASN:ND2	6:E:1561:HOH:O	2.49	0.46
1:F:631:PHE:CG	1:F:632:PRO:HA	2.50	0.46
4:F:805:GOL:H32	6:F:1338:HOH:O	2.15	0.46
1:E:34:LYS:NZ	1:E:355:ASP:OD1	2.49	0.46
1:A:425:LEU:HD12	1:A:622:ILE:HD11	1.98	0.46
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.50	0.46
1:E:328[A]:MET:SD	1:E:402:ALA:HB2	2.55	0.46
1:A:333:SER:HB3	1:A:336:CYS:H	1.80	0.46
1:C:436:ASP:H	4:C:804:GOL:H32	1.79	0.46
4:E:804:GOL:C1	6:E:1656:HOH:O	2.63	0.46
1:F:121:LEU:C	1:F:123:SER:N	2.70	0.45
1:C:335:GLY:CA	1:C:336:CYS:CB	2.93	0.45
1:B:468:ILE:H	1:B:473:ASN:ND2	2.04	0.45
1:E:175[A]:VAL:CG1	1:E:190:LEU:HD12	2.47	0.45
1:D:580:LEU:HD12	4:D:811:GOL:H32	1.99	0.45
1:F:642:MET:CE	6:F:1541:HOH:O	2.65	0.45
1:E:18:PRO:CA	6:E:1230:HOH:O	2.64	0.45
1:B:328[A]:MET:SD	1:B:402:ALA:HA	2.57	0.45
1:E:631:PHE:CG	1:E:632:PRO:HA	2.51	0.45
1:E:343:HIS:ND1	4:E:804:GOL:O2	2.43	0.45
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.47	0.44
1:A:121[A]:LEU:N	1:A:121[A]:LEU:HD12	2.33	0.44
1:A:333:SER:HG	1:A:336:CYS:HB2	1.82	0.44
1:B:175[A]:VAL:CG1	1:B:190:LEU:HD12	2.46	0.44
1:D:644:ARG:NH2	6:D:1511:HOH:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:805:GOL:C3	6:E:1524:HOH:O	2.43	0.44
1:F:670:ARG:C	1:F:672:VAL:H	2.19	0.44
1:A:333:SER:OG	1:A:336:CYS:CB	2.65	0.44
1:A:70:GLN:O	4:A:803:GOL:H2	2.18	0.44
1:D:84:LEU:HD12	1:D:84:LEU:N	2.32	0.44
1:F:305:TYR:OH	1:F:405[B]:TYY:OH	2.29	0.44
1:A:366:HIS:HE1	6:A:1296:HOH:O	2.01	0.43
1:C:375:LYS:HG3	1:C:388[A]:VAL:HG22	2.00	0.43
1:D:18:PRO:CA	4:D:808:GOL:O1	2.66	0.43
1:A:374:PHE:CD1	1:B:633:LEU:HD13	2.53	0.43
1:B:334:LEU:HD23	1:B:334:LEU:O	2.18	0.43
1:D:328[B]:MET:HE3	6:D:1177:HOH:O	1.90	0.43
1:C:286:HIS:HE1	6:C:947:HOH:O	2.02	0.43
1:C:333:SER:N	1:C:337:ASP:OD2	2.52	0.43
1:D:328[A]:MET:SD	1:D:402:ALA:HB2	2.58	0.43
1:A:66:GLN:HG3	1:A:70:GLN:NE2	2.34	0.43
1:F:202:LYS:NZ	6:F:1252:HOH:O	2.51	0.43
1:F:265:LYS:HE2	4:F:803:GOL:H2	2.00	0.43
1:C:644:ARG:HD2	6:C:1338:HOH:O	2.19	0.43
1:C:286:HIS:HD2	6:D:1656:HOH:O	2.01	0.43
1:B:301:MET:O	1:B:318:LEU:HA	2.18	0.43
1:D:147:GLU:OE1	4:D:803:GOL:O3	2.36	0.43
1:E:395:VAL:HG12	1:E:397[A]:SER:OG	2.18	0.43
1:C:175[B]:VAL:HG13	1:C:190:LEU:HB2	2.00	0.43
1:C:405[A]:TYY:CZ	6:C:1241:HOH:O	2.43	0.43
1:C:631:PHE:CG	1:C:632:PRO:HA	2.54	0.43
1:C:218:HIS:HD2	5:C:808:PO4:O3	2.02	0.42
1:E:121:LEU:CB	6:E:1659:HOH:O	2.64	0.42
1:A:47:LYS:HE3	6:A:1406:HOH:O	2.19	0.42
1:D:366:HIS:CD2	1:D:368:GLU:HG3	2.54	0.42
1:F:335:GLY:O	1:F:336:CYS:C	2.55	0.42
1:C:333:SER:HB2	1:C:335:GLY:N	2.35	0.42
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.49	0.42
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.55	0.42
1:E:222:ASN:HB3	1:E:227:HIS:CG	2.54	0.42
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.55	0.42
1:C:84:LEU:HD12	1:C:84:LEU:N	2.35	0.42
1:E:366:HIS:CE1	6:E:1359:HOH:O	2.72	0.42
1:B:375:LYS:HE3	1:B:388:VAL:HG22	2.01	0.42
1:C:120:ASP:HB3	1:C:352:ARG:NH2	2.27	0.42
1:A:375:LYS:NZ	1:B:330:ASN:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:O	4:B:804:GOL:O2	2.38	0.42
1:C:121[A]:LEU:HD23	1:C:171:GLN:OE1	2.19	0.41
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.55	0.41
1:F:66:GLN:NE2	6:F:1344:HOH:O	2.53	0.41
1:D:222:ASN:HB3	1:D:227:HIS:CG	2.55	0.41
1:E:118:VAL:O	1:E:119:GLU:C	2.56	0.41
1:E:308:PRO:HB3	1:F:497:ALA:HB2	2.02	0.41
1:A:330:ASN:HD22	1:B:375:LYS:NZ	2.18	0.41
1:D:41:LYS:CE	6:D:943:HOH:O	2.69	0.41
1:A:670:ARG:C	1:A:672:VAL:H	2.24	0.41
1:A:323:TYR:HB2	1:A:328[A]:MET:CE	2.50	0.41
1:A:324:GLY:N	1:A:328[A]:MET:HE2	2.36	0.41
1:F:402:ALA:HB3	1:F:405[A]:TYY:HD2	2.03	0.41
1:D:342:ILE:HG22	1:D:366:HIS:HB3	2.02	0.41
1:E:175[A]:VAL:HG11	1:E:190:LEU:HD12	2.03	0.41
1:E:68:LYS:HD3	1:E:69:GLU:HG3	2.03	0.41
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.51	0.41
1:A:308:PRO:HB3	1:B:497:ALA:HB2	2.03	0.41
1:C:333:SER:HB3	1:C:335:GLY:HA3	2.00	0.41
1:E:375:LYS:HZ3	1:F:330:ASN:HD22	1.68	0.40
1:A:425:LEU:CD1	1:A:622:ILE:HD11	2.51	0.40
1:B:323:TYR:HB2	1:B:328[A]:MET:CE	2.51	0.40
1:C:121[B]:LEU:CG	1:C:155:PRO:HG2	2.49	0.40
1:D:252:PHE:HB2	1:D:259:MET:SD	2.61	0.40
1:A:342:ILE:HG21	1:A:364:CYS:HB2	2.04	0.40
1:A:328[A]:MET:SD	1:A:402:ALA:HA	2.62	0.40
1:B:506:LYS:HD2	6:B:1309:HOH:O	2.20	0.40
1:C:407:TYR:CD1	1:C:425:LEU:HD22	2.56	0.40
1:E:382:ASN:CB	6:E:1561:HOH:O	2.69	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	658/692 (95%)	636 (97%)	20 (3%)	2 (0%)	41	24
1	B	658/692 (95%)	638 (97%)	18 (3%)	2 (0%)	41	24
1	C	662/692 (96%)	638 (96%)	21 (3%)	3 (0%)	29	13
1	D	660/692 (95%)	640 (97%)	18 (3%)	2 (0%)	41	24
1	E	657/692 (95%)	635 (97%)	21 (3%)	1 (0%)	47	30
1	F	660/692 (95%)	637 (96%)	19 (3%)	4 (1%)	25	11
All	All	3955/4152 (95%)	3824 (97%)	117 (3%)	14 (0%)	34	18

All (14) 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
1	D	671	ALA
1	F	122	CYS
1	F	336	CYS
1	B	334	LEU
1	B	155	PRO
1	D	155	PRO
1	E	155	PRO
1	A	155	PRO
1	F	155	PRO

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	570/593 (96%)	565 (99%)	5 (1%)	78	70
1	B	570/593 (96%)	563 (99%)	7 (1%)	71	59
1	C	575/593 (97%)	572 (100%)	3 (0%)	88	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	573/593 (97%)	568 (99%)	5 (1%)	78	70
1	E	570/593 (96%)	563 (99%)	7 (1%)	71	59
1	F	572/593 (96%)	567 (99%)	5 (1%)	78	70
All	All	3430/3558 (96%)	3398 (99%)	32 (1%)	78	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	THR
1	A	333	SER
1	A	334	LEU
1	A	364	CYS
1	A	633	LEU
1	B	84	LEU
1	B	114	PRO
1	B	329	THR
1	B	334	LEU
1	B	369[A]	ASP
1	B	369[B]	ASP
1	B	633	LEU
1	C	240	PRO
1	C	329	THR
1	C	333	SER
1	D	109	LEU
1	D	213	ARG
1	D	217	LYS
1	D	329	THR
1	D	339	LYS
1	E	48	LYS
1	E	84	LEU
1	E	109	LEU
1	E	126	GLU
1	E	213	ARG
1	E	329	THR
1	E	339	LYS
1	F	76	PRO
1	F	231	LYS
1	F	311	PRO
1	F	329	THR
1	F	334	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	171	GLN
1	A	218	HIS
1	A	286	HIS
1	A	312	HIS
1	A	330	ASN
1	A	361	ASN
1	A	366	HIS
1	A	398	GLN
1	A	547	GLN
1	B	70	GLN
1	B	171	GLN
1	B	286	HIS
1	B	330	ASN
1	B	361	ASN
1	B	366	HIS
1	B	398	GLN
1	B	450	ASN
1	B	473	ASN
1	C	70	GLN
1	C	218	HIS
1	C	286	HIS
1	C	330	ASN
1	C	348	HIS
1	C	361	ASN
1	C	398	GLN
1	D	343	HIS
1	D	361	ASN
1	D	398	GLN
1	E	330	ASN
1	E	348	HIS
1	E	361	ASN
1	E	382	ASN
1	E	398	GLN
1	F	330	ASN
1	F	361	ASN
1	F	398	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	F	405[B]	1	11,14,15	1.63	3 (27%)	13,19,21	2.09	3 (23%)
1	TYY	C	405[B]	1	11,14,15	1.42	1 (9%)	13,19,21	2.20	2 (15%)
1	TYY	F	405[A]	1	11,14,15	1.68	2 (18%)	13,19,21	1.97	4 (30%)
1	TYY	C	405[A]	1	11,14,15	1.73	2 (18%)	13,19,21	1.77	5 (38%)
1	TYY	D	405	1	11,14,15	2.49	3 (27%)	13,19,21	2.63	4 (30%)
1	TYY	A	405	1	11,14,15	2.25	5 (45%)	13,19,21	2.53	6 (46%)
1	TYY	B	405	1	11,14,15	2.32	4 (36%)	13,19,21	2.47	5 (38%)
1	TYY	E	405	1	11,14,15	2.39	4 (36%)	13,19,21	2.89	5 (38%)

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	F	405[B]	1	-	1/5/22/24	0/1/1/1
1	TYY	C	405[B]	1	-	2/5/22/24	0/1/1/1
1	TYY	F	405[A]	1	-	0/5/22/24	0/1/1/1
1	TYY	C	405[A]	1	-	0/5/22/24	0/1/1/1
1	TYY	D	405	1	-	1/5/22/24	0/1/1/1
1	TYY	A	405	1	-	0/5/22/24	0/1/1/1
1	TYY	B	405	1	-	0/5/22/24	0/1/1/1
1	TYY	E	405	1	-	1/5/22/24	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405	TYY	CE1-CZ	5.21	1.43	1.35
1	E	405	TYY	CE1-CZ	4.93	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	TYY	CD2-CG	4.03	1.45	1.34
1	D	405	TYY	CD2-CG	3.93	1.44	1.34
1	B	405	TYY	CE1-CZ	3.62	1.41	1.35
1	D	405	TYY	CG-CD1	-3.54	1.43	1.49
1	C	405[A]	TYY	CE1-CZ	3.46	1.41	1.35
1	A	405	TYY	CD2-CE2	-3.44	1.36	1.43
1	B	405	TYY	CD2-CG	3.36	1.43	1.34
1	B	405	TYY	OZ-CD1	3.28	1.33	1.24
1	F	405[A]	TYY	CE1-CZ	3.28	1.40	1.35
1	A	405	TYY	CE1-CZ	3.28	1.40	1.35
1	A	405	TYY	CD2-CG	3.07	1.42	1.34
1	A	405	TYY	OZ-CD1	3.00	1.32	1.24
1	E	405	TYY	OZ-CD1	2.80	1.32	1.24
1	B	405	TYY	CD2-CE2	-2.76	1.38	1.43
1	E	405	TYY	CG-CD1	-2.63	1.45	1.49
1	C	405[B]	TYY	CG-CD1	-2.45	1.45	1.49
1	F	405[A]	TYY	OZ-CD1	2.42	1.31	1.24
1	F	405[B]	TYY	CD2-CE2	-2.37	1.38	1.43
1	F	405[B]	TYY	CB-CA	-2.30	1.48	1.53
1	F	405[B]	TYY	OZ-CD1	2.26	1.30	1.24
1	A	405	TYY	OH-CZ	2.24	1.39	1.34
1	C	405[A]	TYY	CB-CG	2.02	1.54	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	405	TYY	CD2-CG-CD1	7.61	124.49	118.64
1	D	405	TYY	CD2-CG-CD1	6.49	123.63	118.64
1	F	405[B]	TYY	CB-CA-C	-6.08	100.08	111.47
1	C	405[B]	TYY	CB-CA-C	-5.54	101.08	111.47
1	B	405	TYY	CB-CA-C	-5.48	101.19	111.47
1	A	405	TYY	CB-CA-C	-4.81	102.45	111.47
1	D	405	TYY	CB-CA-C	-4.65	102.74	111.47
1	E	405	TYY	CB-CA-C	-4.28	103.44	111.47
1	B	405	TYY	CD2-CG-CD1	4.09	121.78	118.64
1	A	405	TYY	CZ-CE1-CD1	4.09	124.83	120.30
1	F	405[A]	TYY	CB-CA-C	-4.04	103.89	111.47
1	C	405[B]	TYY	CD2-CG-CD1	3.86	121.61	118.64
1	E	405	TYY	CD2-CE2-CZ	-3.81	113.89	117.91
1	F	405[A]	TYY	CZ-CE1-CD1	3.63	124.33	120.30
1	A	405	TYY	CD2-CE2-CZ	-3.53	114.19	117.91
1	D	405	TYY	CD2-CE2-CZ	-3.38	114.35	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	TYY	CZ-CE1-CD1	3.31	123.97	120.30
1	A	405	TYY	CE2-CD2-CG	3.22	125.73	120.62
1	F	405[B]	TYY	CD2-CG-CD1	3.08	121.00	118.64
1	C	405[A]	TYY	CB-CA-C	-3.07	105.72	111.47
1	C	405[A]	TYY	CZ-CE1-CD1	2.91	123.52	120.30
1	A	405	TYY	CD2-CG-CD1	2.87	120.84	118.64
1	C	405[A]	TYY	CE1-CZ-CE2	-2.76	118.11	121.75
1	F	405[A]	TYY	CE1-CZ-CE2	-2.69	118.20	121.75
1	B	405	TYY	CD2-CE2-CZ	-2.60	115.17	117.91
1	F	405[A]	TYY	CE2-CD2-CG	2.41	124.46	120.62
1	F	405[B]	TYY	CZ-CE1-CD1	2.34	122.89	120.30
1	C	405[A]	TYY	CE2-CD2-CG	2.32	124.31	120.62
1	E	405	TYY	CA-CB-CG	2.31	117.92	113.51
1	D	405	TYY	CA-CB-CG	2.26	117.83	113.51
1	E	405	TYY	CZ-CE1-CD1	2.18	122.72	120.30
1	A	405	TYY	CE1-CD1-CG	-2.12	113.44	118.46
1	C	405[A]	TYY	CB-CG-CD1	2.10	122.34	118.57
1	B	405	TYY	OH-CZ-CE2	-2.08	113.77	117.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	405[B]	TYY	O-C-CA-CB
1	C	405[B]	TYY	N-CA-CB-CG
1	D	405	TYY	O-C-CA-CB
1	E	405	TYY	O-C-CA-CB
1	F	405[B]	TYY	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	405[B]	TYY	4	0
1	C	405[B]	TYY	3	0
1	F	405[A]	TYY	8	0
1	C	405[A]	TYY	7	0
1	D	405	TYY	2	0
1	E	405	TYY	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 6 are monoatomic - leaving 61 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	$\# Z > 2$
4	GOL	F	810	-	5,5,5	0.64	0	5,5,5	0.59	0
4	GOL	E	805	-	5,5,5	0.33	0	5,5,5	0.52	0
4	GOL	D	807	-	5,5,5	0.55	0	5,5,5	1.13	0
4	GOL	F	807	-	5,5,5	0.24	0	5,5,5	1.47	1 (20%)
4	GOL	C	809	-	5,5,5	0.99	0	5,5,5	0.98	0
4	GOL	A	804	-	5,5,5	1.01	0	5,5,5	1.31	0
4	GOL	A	809	-	5,5,5	0.34	0	5,5,5	0.66	0
4	GOL	B	809	-	5,5,5	0.54	0	5,5,5	1.41	0
4	GOL	A	807	-	5,5,5	0.69	0	5,5,5	1.65	1 (20%)
4	GOL	B	805	-	5,5,5	0.32	0	5,5,5	0.67	0
3	PEO	D	802	2	1,1,1	4.50	1 (100%)	-	-	-
4	GOL	D	806	-	5,5,5	0.39	0	5,5,5	1.12	0
4	GOL	E	806	-	5,5,5	0.59	0	5,5,5	1.79	1 (20%)
4	GOL	C	805	-	5,5,5	0.41	0	5,5,5	0.72	0
4	GOL	A	805	-	5,5,5	0.63	0	5,5,5	0.90	0
4	GOL	D	810	-	5,5,5	0.33	0	5,5,5	0.55	0
4	GOL	B	807	-	5,5,5	0.79	0	5,5,5	0.44	0
4	GOL	A	812	-	5,5,5	0.51	0	5,5,5	0.47	0
4	GOL	F	804	-	5,5,5	0.45	0	5,5,5	0.77	0
4	GOL	D	809	-	5,5,5	0.18	0	5,5,5	1.47	1 (20%)
4	GOL	D	804	-	5,5,5	0.51	0	5,5,5	0.35	0
5	PO4	C	808	-	4,4,4	1.15	0	6,6,6	1.31	1 (16%)
4	GOL	E	803	-	5,5,5	0.16	0	5,5,5	0.72	0
4	GOL	E	804	-	5,5,5	1.05	0	5,5,5	1.42	1 (20%)
4	GOL	C	807	-	5,5,5	0.38	0	5,5,5	0.73	0
4	GOL	A	803	-	5,5,5	0.96	0	5,5,5	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	803	-	5,5,5	0.61	0	5,5,5	0.81	0
4	GOL	F	811	-	5,5,5	0.63	0	5,5,5	0.44	0
3	PEO	C	802	2	1,1,1	4.69	1 (100%)	-		
4	GOL	F	806	-	5,5,5	0.44	0	5,5,5	1.35	1 (20%)
4	GOL	A	811	-	5,5,5	0.50	0	5,5,5	1.30	1 (20%)
4	GOL	D	808	-	5,5,5	0.38	0	5,5,5	0.73	0
5	PO4	F	808	-	4,4,4	0.72	0	6,6,6	0.88	0
4	GOL	B	808	-	5,5,5	0.80	0	5,5,5	1.01	0
4	GOL	F	803	-	5,5,5	0.53	0	5,5,5	0.80	0
4	GOL	B	804	-	5,5,5	0.55	0	5,5,5	1.95	1 (20%)
4	GOL	C	804	-	5,5,5	0.77	0	5,5,5	0.44	0
4	GOL	A	814	-	5,5,5	0.38	0	5,5,5	0.64	0
4	GOL	A	813	-	5,5,5	0.45	0	5,5,5	0.84	0
5	PO4	B	810	-	4,4,4	0.95	0	6,6,6	0.62	0
4	GOL	E	807	-	5,5,5	0.32	0	5,5,5	2.25	2 (40%)
4	GOL	F	805	-	5,5,5	0.42	0	5,5,5	0.85	0
4	GOL	D	811	-	5,5,5	0.55	0	5,5,5	0.61	0
4	GOL	A	808	-	5,5,5	0.94	0	5,5,5	0.45	0
4	GOL	B	806	-	5,5,5	0.49	0	5,5,5	1.17	0
3	PEO	B	802	2	1,1,1	4.17	1 (100%)	-		
3	PEO	A	802	2	1,1,1	4.64	1 (100%)	-		
4	GOL	B	811	-	5,5,5	0.43	0	5,5,5	0.57	0
4	GOL	C	811	-	5,5,5	0.82	0	5,5,5	0.75	0
4	GOL	D	803	-	5,5,5	0.30	0	5,5,5	1.00	0
4	GOL	B	803	-	5,5,5	0.59	0	5,5,5	0.80	0
4	GOL	F	809	-	5,5,5	0.35	0	5,5,5	0.59	0
3	PEO	E	802	2	1,1,1	4.44	1 (100%)	-		
4	GOL	C	806	-	5,5,5	0.42	0	5,5,5	0.48	0
4	GOL	F	812	-	5,5,5	0.97	0	5,5,5	1.21	0
4	GOL	A	810	-	5,5,5	0.33	0	5,5,5	0.43	0
4	GOL	E	808	-	5,5,5	0.48	0	5,5,5	0.75	0
4	GOL	C	810	-	5,5,5	0.33	0	5,5,5	0.43	0
3	PEO	F	802	2	1,1,1	5.04	1 (100%)	-		
4	GOL	D	805	-	5,5,5	0.31	0	5,5,5	0.73	0
4	GOL	A	806	-	5,5,5	0.37	0	5,5,5	0.99	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
4	GOL	F	810	-	-	2/4/4/4	-
4	GOL	E	805	-	-	2/4/4/4	-
4	GOL	D	807	-	-	2/4/4/4	-
4	GOL	F	807	-	-	1/4/4/4	-
4	GOL	C	809	-	-	0/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-
4	GOL	A	809	-	-	1/4/4/4	-
4	GOL	B	809	-	-	2/4/4/4	-
4	GOL	A	807	-	-	2/4/4/4	-
4	GOL	B	805	-	-	2/4/4/4	-
4	GOL	D	806	-	-	2/4/4/4	-
4	GOL	E	806	-	-	2/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	D	810	-	-	3/4/4/4	-
4	GOL	B	807	-	-	0/4/4/4	-
4	GOL	A	812	-	-	2/4/4/4	-
4	GOL	F	804	-	-	1/4/4/4	-
4	GOL	D	809	-	-	2/4/4/4	-
4	GOL	D	804	-	-	4/4/4/4	-
4	GOL	E	803	-	-	4/4/4/4	-
4	GOL	E	804	-	-	2/4/4/4	-
4	GOL	C	807	-	-	4/4/4/4	-
4	GOL	A	803	-	-	3/4/4/4	-
4	GOL	C	803	-	-	0/4/4/4	-
4	GOL	F	811	-	-	0/4/4/4	-
4	GOL	F	806	-	-	2/4/4/4	-
4	GOL	A	811	-	-	0/4/4/4	-
4	GOL	D	808	-	-	4/4/4/4	-
4	GOL	B	808	-	-	2/4/4/4	-
4	GOL	F	803	-	-	2/4/4/4	-
4	GOL	B	804	-	-	3/4/4/4	-
4	GOL	C	804	-	-	1/4/4/4	-
4	GOL	A	814	-	-	2/4/4/4	-
4	GOL	A	813	-	-	2/4/4/4	-
4	GOL	E	807	-	-	4/4/4/4	-
4	GOL	F	805	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	811	-	-	0/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	C	806	-	-	2/4/4/4	-
4	GOL	B	811	-	-	0/4/4/4	-
4	GOL	C	811	-	-	0/4/4/4	-
4	GOL	D	803	-	-	2/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	F	809	-	-	2/4/4/4	-
4	GOL	F	812	-	-	3/4/4/4	-
4	GOL	A	810	-	-	0/4/4/4	-
4	GOL	E	808	-	-	2/4/4/4	-
4	GOL	C	810	-	-	4/4/4/4	-
4	GOL	D	805	-	-	4/4/4/4	-
4	GOL	A	806	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	PEO	O2-O1	-5.04	0.91	1.42
3	C	802	PEO	O2-O1	-4.69	0.94	1.42
3	A	802	PEO	O2-O1	-4.64	0.95	1.42
3	D	802	PEO	O2-O1	-4.50	0.96	1.42
3	E	802	PEO	O2-O1	-4.44	0.97	1.42
3	B	802	PEO	O2-O1	-4.17	1.00	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	GOL	O1-C1-C2	-3.94	91.30	110.20
4	E	807	GOL	O1-C1-C2	-3.84	91.79	110.20
4	F	807	GOL	O1-C1-C2	-3.10	95.32	110.20
4	E	807	GOL	O2-C2-C3	2.90	121.90	109.12
4	D	809	GOL	O1-C1-C2	-2.84	96.56	110.20
5	C	808	PO4	O4-P-O3	2.60	116.33	107.97
4	F	806	GOL	C3-C2-C1	-2.49	102.04	111.70
4	E	804	GOL	O2-C2-C1	-2.40	98.55	109.12
4	A	811	GOL	C3-C2-C1	-2.31	102.72	111.70
4	A	807	GOL	C3-C2-C1	2.23	120.38	111.70
4	E	806	GOL	O2-C2-C1	-2.20	99.44	109.12

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	807	GOL	O1-C1-C2-C3
4	A	804	GOL	O1-C1-C2-C3
4	A	804	GOL	C1-C2-C3-O3
4	B	809	GOL	O1-C1-C2-C3
4	B	805	GOL	C1-C2-C3-O3
4	A	805	GOL	C1-C2-C3-O3
4	A	812	GOL	C1-C2-C3-O3
4	D	804	GOL	O1-C1-C2-C3
4	D	804	GOL	C1-C2-C3-O3
4	E	803	GOL	C1-C2-C3-O3
4	E	804	GOL	C1-C2-C3-O3
4	C	807	GOL	O1-C1-C2-C3
4	C	807	GOL	C1-C2-C3-O3
4	A	803	GOL	C1-C2-C3-O3
4	E	808	GOL	C1-C2-C3-O3
4	F	806	GOL	O1-C1-C2-C3
4	A	814	GOL	C1-C2-C3-O3
4	A	814	GOL	O2-C2-C3-O3
4	A	813	GOL	C1-C2-C3-O3
4	E	807	GOL	C1-C2-C3-O3
4	F	805	GOL	O1-C1-C2-C3
4	B	806	GOL	O1-C1-C2-C3
4	D	803	GOL	C1-C2-C3-O3
4	D	803	GOL	O2-C2-C3-O3
4	B	803	GOL	O1-C1-C2-C3
4	D	805	GOL	O1-C1-C2-C3
4	A	806	GOL	O1-C1-C2-C3
4	A	806	GOL	C1-C2-C3-O3
4	D	808	GOL	O2-C2-C3-O3
4	D	806	GOL	O1-C1-C2-O2
4	D	804	GOL	O1-C1-C2-O2
4	E	807	GOL	O2-C2-C3-O3
4	D	805	GOL	O2-C2-C3-O3
4	A	806	GOL	O2-C2-C3-O3
4	D	808	GOL	O1-C1-C2-C3
4	D	808	GOL	C1-C2-C3-O3
4	F	810	GOL	O1-C1-C2-C3
4	E	805	GOL	O1-C1-C2-C3
4	D	806	GOL	O1-C1-C2-C3
4	D	810	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	F	812	GOL	O1-C1-C2-C3
4	F	812	GOL	C1-C2-C3-O3
4	D	809	GOL	C1-C2-C3-O3
4	B	808	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	E	807	GOL	O1-C1-C2-C3
4	F	809	GOL	O1-C1-C2-C3
4	C	810	GOL	O1-C1-C2-C3
4	C	810	GOL	C1-C2-C3-O3
4	D	805	GOL	C1-C2-C3-O3
4	D	808	GOL	O1-C1-C2-O2
4	F	810	GOL	O1-C1-C2-O2
4	A	804	GOL	O1-C1-C2-O2
4	A	804	GOL	O2-C2-C3-O3
4	B	809	GOL	O1-C1-C2-O2
4	A	812	GOL	O2-C2-C3-O3
4	C	807	GOL	O1-C1-C2-O2
4	A	803	GOL	O2-C2-C3-O3
4	F	806	GOL	O1-C1-C2-O2
4	B	804	GOL	O1-C1-C2-O2
4	E	807	GOL	O1-C1-C2-O2
4	F	805	GOL	O1-C1-C2-O2
4	B	806	GOL	O1-C1-C2-O2
4	F	809	GOL	O1-C1-C2-O2
4	C	810	GOL	O1-C1-C2-O2
4	C	810	GOL	O2-C2-C3-O3
4	D	807	GOL	O1-C1-C2-O2
4	B	805	GOL	O2-C2-C3-O3
4	A	805	GOL	O2-C2-C3-O3
4	D	809	GOL	O2-C2-C3-O3
4	D	804	GOL	O2-C2-C3-O3
4	E	803	GOL	O2-C2-C3-O3
4	E	808	GOL	O2-C2-C3-O3
4	A	813	GOL	O2-C2-C3-O3
4	B	803	GOL	O1-C1-C2-O2
4	A	806	GOL	O1-C1-C2-O2
4	A	807	GOL	O1-C1-C2-O2
4	F	804	GOL	O1-C1-C2-O2
4	E	803	GOL	O1-C1-C2-O2
4	E	804	GOL	O2-C2-C3-O3
4	A	803	GOL	O1-C1-C2-O2
4	D	805	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	F	812	GOL	O2-C2-C3-O3
4	C	807	GOL	O2-C2-C3-O3
4	C	806	GOL	O1-C1-C2-O2
4	F	803	GOL	O1-C1-C2-C3
4	E	805	GOL	O1-C1-C2-O2
4	B	808	GOL	O2-C2-C3-O3
4	F	807	GOL	C1-C2-C3-O3
4	D	810	GOL	O2-C2-C3-O3
4	E	806	GOL	C1-C2-C3-O3
4	D	810	GOL	O1-C1-C2-C3
4	E	803	GOL	O1-C1-C2-C3
4	C	804	GOL	O1-C1-C2-C3
4	C	806	GOL	O1-C1-C2-C3
4	F	803	GOL	O1-C1-C2-O2
4	A	807	GOL	O1-C1-C2-C3
4	E	806	GOL	O1-C1-C2-C3
4	B	804	GOL	C1-C2-C3-O3
4	A	809	GOL	O2-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	810	GOL	1	0
4	E	805	GOL	2	0
4	C	809	GOL	1	0
4	A	804	GOL	1	0
5	C	808	PO4	1	0
4	E	804	GOL	3	0
4	A	803	GOL	1	0
4	A	811	GOL	3	0
4	D	808	GOL	5	0
4	F	803	GOL	1	0
4	B	804	GOL	1	0
4	C	804	GOL	1	0
4	F	805	GOL	1	0
4	D	811	GOL	4	0
4	D	803	GOL	1	0
4	C	810	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 ⓘ

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, 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	655/692 (94%)	-0.76	3 (0%)	91 92	7, 12, 27, 71	0
1	B	655/692 (94%)	-0.76	3 (0%)	91 92	7, 12, 27, 72	0
1	C	654/692 (94%)	-0.70	3 (0%)	91 92	8, 13, 30, 69	0
1	D	654/692 (94%)	-0.74	3 (0%)	91 92	8, 13, 29, 78	0
1	E	654/692 (94%)	-0.73	3 (0%)	91 92	7, 13, 29, 80	0
1	F	655/692 (94%)	-0.70	3 (0%)	91 92	7, 13, 30, 66	0
All	All	3927/4152 (94%)	-0.73	18 (0%)	91 92	7, 13, 29, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	672	VAL	5.9
1	C	334	LEU	4.9
1	B	334	LEU	4.7
1	D	672	VAL	4.6
1	C	672	VAL	4.2
1	A	334	LEU	4.0
1	B	672	VAL	3.6
1	F	672	VAL	3.4
1	C	121[A]	LEU	3.3
1	F	334	LEU	3.0
1	E	121	LEU	2.9
1	F	121	LEU	2.5
1	B	22	ALA	2.4
1	A	22	ALA	2.2
1	A	672	VAL	2.2
1	E	18	PRO	2.1
1	D	121	LEU	2.1
1	D	18	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	E	405	14/15	0.95	0.08	10,13,20,25	0
1	TYY	D	405	14/15	0.96	0.07	10,14,21,26	0
1	TYY	B	405	14/15	0.97	0.07	11,13,18,18	0
1	TYY	C	405[A]	14/15	0.98	0.08	9,10,11,11	14
1	TYY	F	405[B]	14/15	0.98	0.09	10,12,13,14	14
1	TYY	A	405	14/15	0.98	0.06	11,12,17,18	0
1	TYY	C	405[B]	14/15	0.98	0.08	11,11,12,12	14
1	TYY	F	405[A]	14/15	0.98	0.09	10,10,11,11	14

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	GOL	D	804	6/6	0.36	0.47	87,97,103,107	0
4	GOL	D	808	6/6	0.73	0.18	46,51,55,58	0
4	GOL	F	812	6/6	0.78	0.14	33,40,41,42	0
4	GOL	B	806	6/6	0.78	0.33	29,34,40,41	6
4	GOL	D	811	6/6	0.80	0.15	39,49,52,54	0
4	GOL	A	805	6/6	0.80	0.12	30,33,39,41	0
4	GOL	C	806	6/6	0.81	0.15	29,32,33,33	0
4	GOL	D	810	6/6	0.82	0.15	50,55,59,68	0
4	GOL	F	810	6/6	0.82	0.19	33,48,50,56	0
4	GOL	C	804	6/6	0.84	0.13	31,39,41,42	0
4	GOL	A	807	6/6	0.84	0.11	38,47,50,51	0
4	GOL	F	805	6/6	0.85	0.13	38,40,42,48	0
4	GOL	A	813	6/6	0.85	0.13	26,38,45,50	0
4	GOL	F	809	6/6	0.86	0.24	38,58,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	804	6/6	0.86	0.11	31,38,39,39	0
4	GOL	D	805	6/6	0.87	0.11	46,48,49,55	0
4	GOL	B	803	6/6	0.88	0.09	34,36,39,41	0
4	GOL	B	808	6/6	0.88	0.12	29,39,43,45	0
4	GOL	E	804	6/6	0.89	0.10	26,37,39,43	0
4	GOL	C	807	6/6	0.89	0.16	39,42,49,50	0
4	GOL	B	805	6/6	0.89	0.11	37,39,41,42	0
4	GOL	A	812	6/6	0.89	0.10	38,42,43,44	0
4	GOL	F	807	6/6	0.90	0.13	34,38,41,49	0
4	GOL	D	803	6/6	0.90	0.13	34,41,43,49	0
4	GOL	A	814	6/6	0.91	0.13	52,60,62,62	0
4	GOL	A	811	6/6	0.91	0.11	30,38,44,44	0
4	GOL	F	804	6/6	0.91	0.12	29,30,32,33	0
4	GOL	B	804	6/6	0.91	0.17	24,38,41,45	0
4	GOL	B	809	6/6	0.91	0.11	27,36,46,48	0
4	GOL	C	810	6/6	0.92	0.10	31,45,50,50	0
4	GOL	A	806	6/6	0.92	0.11	38,45,49,51	0
4	GOL	C	805	6/6	0.93	0.12	39,42,44,46	0
4	GOL	A	809	6/6	0.93	0.09	37,38,40,43	0
4	GOL	E	807	6/6	0.93	0.15	20,29,32,36	0
4	GOL	D	809	6/6	0.93	0.13	22,28,30,33	0
4	GOL	E	805	6/6	0.93	0.12	38,42,47,55	0
4	GOL	E	806	6/6	0.93	0.13	42,47,48,49	0
4	GOL	B	811	6/6	0.93	0.12	38,42,44,51	0
4	GOL	E	808	6/6	0.94	0.10	27,32,35,35	0
5	PO4	B	810	5/5	0.94	0.09	31,35,37,37	5
4	GOL	D	807	6/6	0.94	0.12	27,30,33,34	0
4	GOL	A	810	6/6	0.94	0.12	37,39,42,48	0
4	GOL	C	811	6/6	0.94	0.12	15,18,20,21	0
4	GOL	A	803	6/6	0.94	0.09	15,21,26,33	0
5	PO4	F	808	5/5	0.94	0.12	33,46,51,52	0
4	GOL	E	803	6/6	0.95	0.13	31,37,41,44	0
4	GOL	F	806	6/6	0.95	0.10	24,32,40,42	0
5	PO4	C	808	5/5	0.95	0.15	31,43,47,48	0
4	GOL	F	811	6/6	0.96	0.11	15,19,20,20	0
4	GOL	B	807	6/6	0.96	0.13	15,17,18,20	0
4	GOL	C	809	6/6	0.96	0.08	15,20,20,28	0
4	GOL	D	806	6/6	0.96	0.07	19,30,33,36	0
4	GOL	F	803	6/6	0.96	0.10	19,25,28,34	0
4	GOL	C	803	6/6	0.97	0.12	19,26,29,33	0
3	PEO	E	802	2/2	0.98	0.10	6,6,6,10	0
4	GOL	A	808	6/6	0.98	0.11	14,16,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEO	D	802	2/2	0.98	0.11	6,6,6,10	0
3	PEO	F	802	2/2	0.99	0.07	7,7,7,9	0
3	PEO	B	802	2/2	0.99	0.10	5,5,5,11	0
3	PEO	A	802	2/2	0.99	0.08	7,7,7,10	0
2	CU	C	801	1/1	1.00	0.04	11,11,11,11	0
2	CU	B	801	1/1	1.00	0.06	12,12,12,12	0
2	CU	E	801	1/1	1.00	0.04	11,11,11,11	0
2	CU	D	801	1/1	1.00	0.04	11,11,11,11	0
3	PEO	C	802	2/2	1.00	0.06	8,8,8,8	0
2	CU	A	801	1/1	1.00	0.06	12,12,12,12	0
2	CU	F	801	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.