wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2024 – 09:09 AM EDT

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

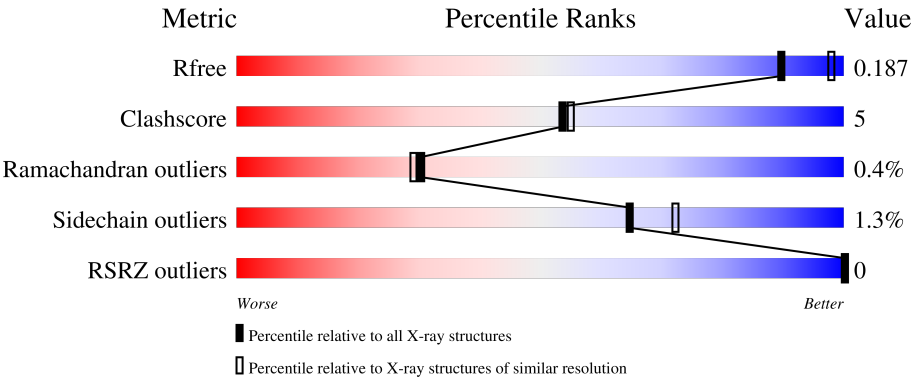
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	692	85% 9% • 5%
1	B	692	85% 9% 5%
1	C	692	86% 8% • 5%
1	D	692	86% 8% • 5%
1	E	692	85% 9% • 5%

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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
5	GOL	D	711	-	-	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.

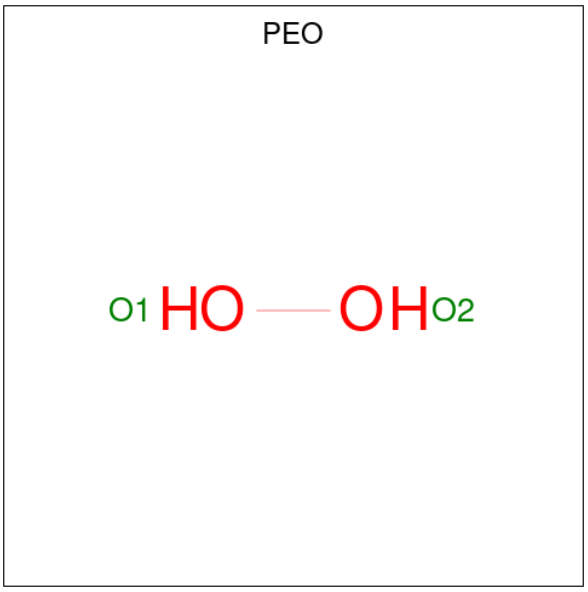
- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

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).

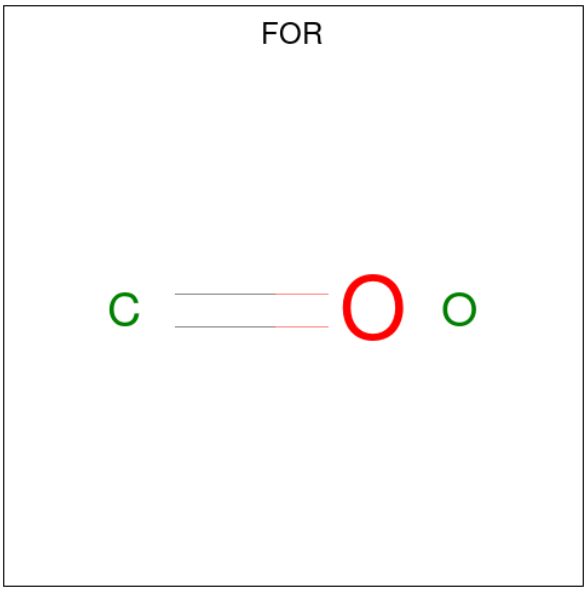
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



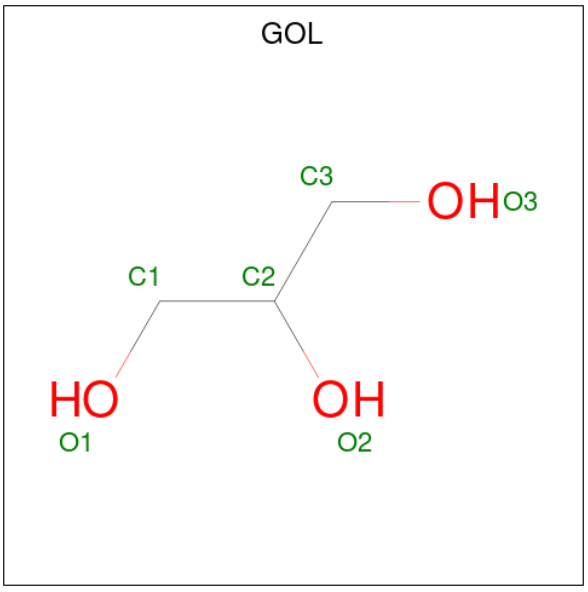
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	E	1	Total O 2 2	0	0
3	F	1	Total O 2 2	0	0

- Molecule 4 is FORMYL GROUP (three-letter code: FOR) (formula: CH_2O).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

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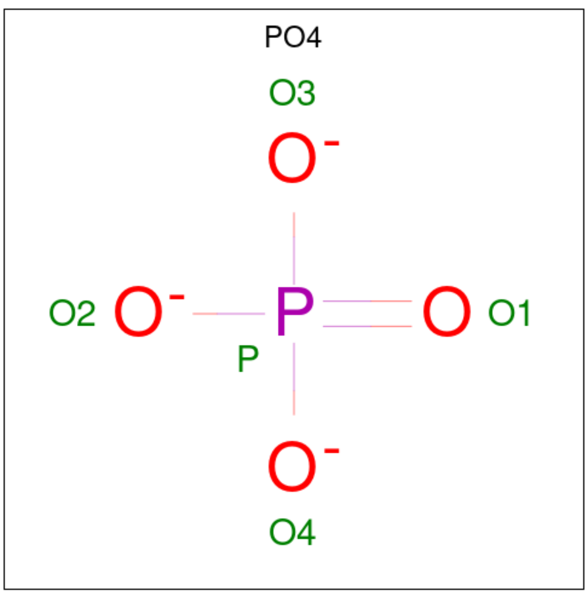
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

- Molecule 7 is water.

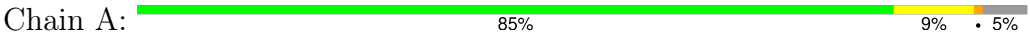
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	757	Total O 757 757	0	0
7	B	734	Total O 734 734	0	0
7	C	727	Total O 727 727	0	0
7	D	732	Total O 732 732	0	0
7	E	726	Total O 726 726	0	0
7	F	709	Total O 709 709	0	0

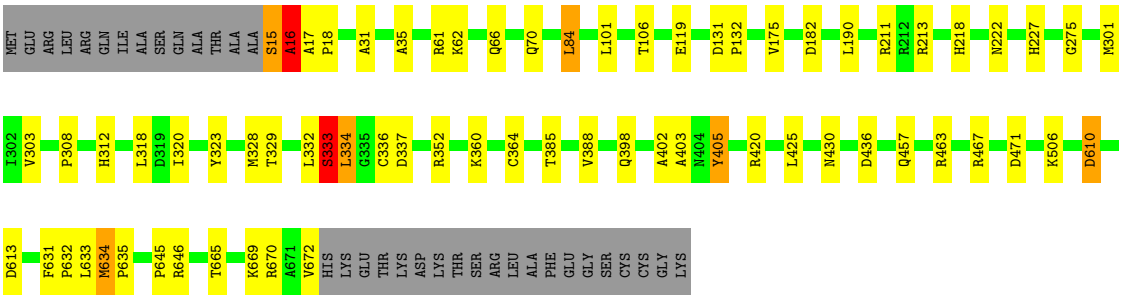
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Peroxisomal primary amine oxidase

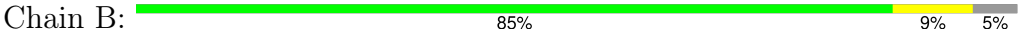
Chain A:

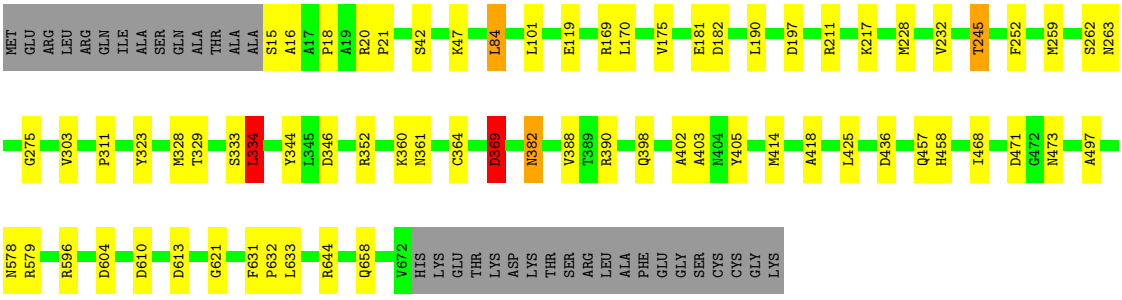




• Molecule 1: Peroxisomal primary amine oxidase

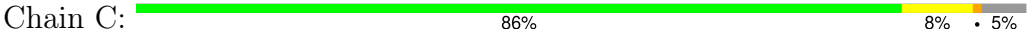
Chain B:

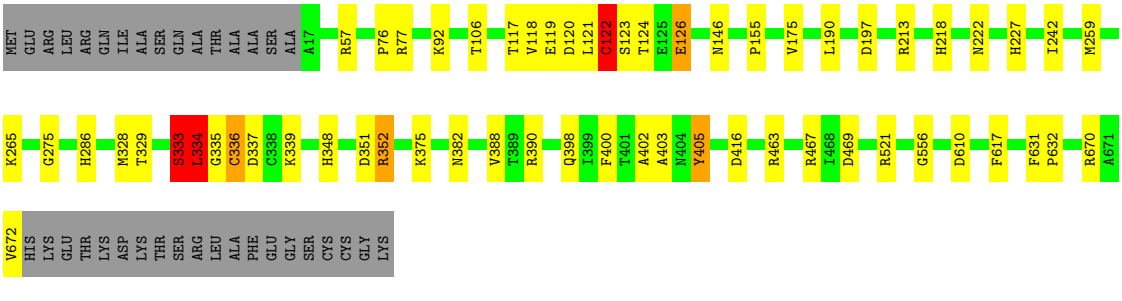




• Molecule 1: Peroxisomal primary amine oxidase

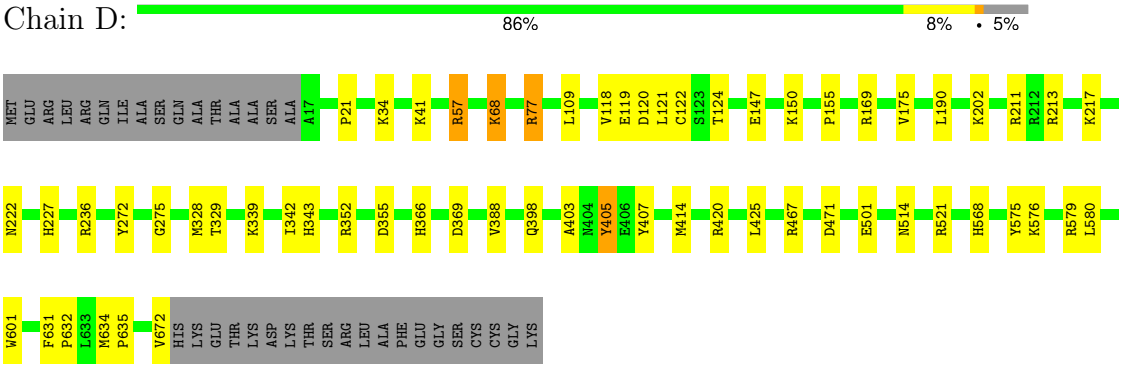
Chain C:





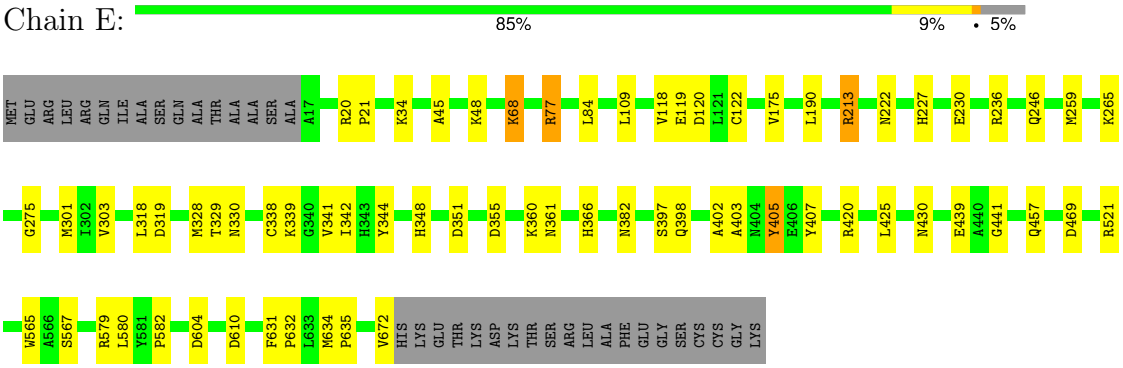
• Molecule 1: Peroxisomal primary amine oxidase

Chain D:



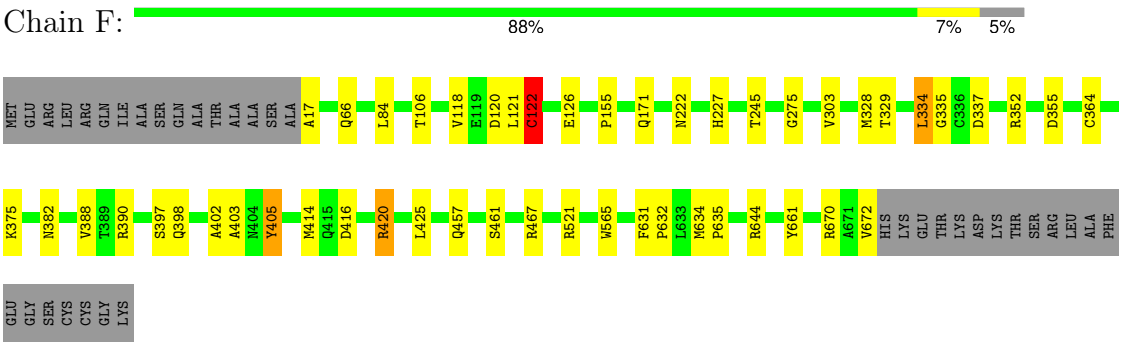
• Molecule 1: Peroxisomal primary amine oxidase

Chain E:



• Molecule 1: Peroxisomal primary amine oxidase

Chain F:



4 Data and refinement statistics (i)

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)	49.03 – 2.10 49.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.03-2.10) 98.5 (49.03-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	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	13291 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.479 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	36172	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FOR, TYY, GOL, PO4, PEO, 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(^{o})	Ideal(^{o})
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%)	25	23
1	B	659/692 (95%)	637 (97%)	20 (3%)	2 (0%)	37	37
1	C	663/692 (96%)	633 (96%)	25 (4%)	5 (1%)	16	13
1	D	662/692 (96%)	638 (96%)	22 (3%)	2 (0%)	37	37
1	E	658/692 (95%)	637 (97%)	20 (3%)	1 (0%)	44	45
1	F	660/692 (95%)	634 (96%)	23 (4%)	3 (0%)	25	23
All	All	3962/4152 (95%)	3814 (96%)	132 (3%)	16 (0%)	30	29

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%)	58	65
1	B	570/593 (96%)	558 (98%)	12 (2%)	48	55
1	C	575/593 (97%)	571 (99%)	4 (1%)	81	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	574/593 (97%)	565 (98%)	9 (2%)	58 65
1	E	570/593 (96%)	560 (98%)	10 (2%)	54 61
1	F	572/593 (96%)	569 (100%)	3 (0%)	86 91
All	All	3431/3558 (96%)	3384 (99%)	47 (1%)	65 70

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

Mol	Chain	Res	Type
1	D	213	ARG
1	E	68	LYS
1	D	217	LYS
1	D	369[A]	ASP
1	E	109	LEU

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

Mol	Chain	Res	Type
1	D	210	ASN
1	E	348	HIS
1	D	343	HIS
1	E	70	GLN
1	E	398	GLN

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	1	13,14,15	3.05	7 (53%)	10,19,21	1.47	2 (20%)
1	TYY	B	405	1	13,14,15	2.94	6 (46%)	10,19,21	1.24	1 (10%)
1	TYY	D	405	1	13,14,15	2.51	5 (38%)	10,19,21	1.52	2 (20%)
1	TYY	E	405	1	13,14,15	2.93	5 (38%)	10,19,21	1.83	2 (20%)
1	TYY	C	405	1	13,14,15	2.65	5 (38%)	10,19,21	1.67	3 (30%)
1	TYY	F	405	1	13,14,15	2.38	6 (46%)	10,19,21	1.76	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	1	-	0/5/22/24	0/1/1/1
1	TYY	B	405	1	-	1/5/22/24	0/1/1/1
1	TYY	D	405	1	-	0/5/22/24	0/1/1/1
1	TYY	E	405	1	-	1/5/22/24	0/1/1/1
1	TYY	C	405	1	-	1/5/22/24	0/1/1/1
1	TYY	F	405	1	-	0/5/22/24	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	TYY	CE2-N5	8.44	1.42	1.28
1	A	405	TYY	CE2-N5	8.36	1.41	1.28
1	B	405	TYY	CE2-N5	7.86	1.41	1.28
1	C	405	TYY	CE2-N5	6.87	1.39	1.28
1	D	405	TYY	CE2-N5	6.54	1.38	1.28

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	405	TYY	CD2-CG-CD1	3.77	121.34	118.66
1	C	405	TYY	CE1-CZ-CE2	-3.55	117.61	122.00
1	E	405	TYY	CZ-CE1-CD1	3.34	123.92	120.30
1	A	405	TYY	CD2-CG-CD1	3.08	120.85	118.66
1	D	405	TYY	OZ-CD1-CG	-3.00	114.98	120.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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	D	405	TYY	3	0
1	E	405	TYY	2	0
1	C	405	TYY	4	0
1	F	405	TYY	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
5	GOL	C	803	-	5,5,5	0.35	0	5,5,5	0.62	0
5	GOL	B	804	-	5,5,5	0.39	0	5,5,5	0.88	0
5	GOL	E	806	-	5,5,5	0.24	0	5,5,5	1.37	1 (20%)
5	GOL	F	810	-	5,5,5	0.30	0	5,5,5	0.56	0
5	GOL	F	805	-	5,5,5	0.29	0	5,5,5	0.66	0
5	GOL	D	707	-	5,5,5	0.44	0	5,5,5	1.20	0
6	PO4	C	808	-	4,4,4	1.01	0	6,6,6	0.93	0
5	GOL	A	812	-	5,5,5	0.29	0	5,5,5	0.42	0
5	GOL	F	808	-	5,5,5	0.27	0	5,5,5	0.68	0
5	GOL	D	708	-	5,5,5	0.26	0	5,5,5	1.49	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	C	804	-	5,5,5	0.92	0	5,5,5	0.61	0
5	GOL	B	813	-	5,5,5	0.32	0	5,5,5	0.47	0
5	GOL	C	807	-	5,5,5	0.26	0	5,5,5	1.08	0
3	PEO	F	802	2	1,1,1	1.18	0	-		
4	FOR	D	702	-	0,1,1	-	-	-		
5	GOL	A	810	-	5,5,5	0.42	0	5,5,5	1.00	0
5	GOL	A	815	-	5,5,5	0.29	0	5,5,5	0.86	0
5	GOL	E	804	-	5,5,5	0.76	0	5,5,5	0.64	0
5	GOL	A	816	-	5,5,5	0.46	0	5,5,5	0.54	0
5	GOL	E	807	-	5,5,5	0.40	0	5,5,5	1.03	1 (20%)
3	PEO	A	802	2	1,1,1	0.97	0	-		
5	GOL	C	805	-	5,5,5	0.60	0	5,5,5	0.99	0
3	PEO	B	802	2	1,1,1	0.87	0	-		
5	GOL	A	806	-	5,5,5	0.53	0	5,5,5	1.21	1 (20%)
5	GOL	A	807	-	5,5,5	0.36	0	5,5,5	1.02	0
6	PO4	F	809	-	4,4,4	0.70	0	6,6,6	0.86	0
5	GOL	D	711	-	5,5,5	0.76	0	5,5,5	0.78	0
5	GOL	D	710	-	5,5,5	0.28	0	5,5,5	0.23	0
5	GOL	B	807	-	5,5,5	0.25	0	5,5,5	0.68	0
5	GOL	E	803	-	5,5,5	0.31	0	5,5,5	1.07	0
5	GOL	F	811	-	5,5,5	0.92	0	5,5,5	0.62	0
5	GOL	A	814	-	5,5,5	0.62	0	5,5,5	0.59	0
5	GOL	A	808	-	5,5,5	0.43	0	5,5,5	1.12	0
5	GOL	D	709	-	5,5,5	0.29	0	5,5,5	0.65	0
5	GOL	A	804	-	5,5,5	0.72	0	5,5,5	0.95	0
5	GOL	B	805	-	5,5,5	0.63	0	5,5,5	1.66	2 (40%)
5	GOL	C	809	-	5,5,5	0.73	0	5,5,5	0.46	0
3	PEO	D	701	2	1,1,1	1.19	0	-		
5	GOL	F	807	-	5,5,5	0.64	0	5,5,5	0.86	0
5	GOL	B	808	-	5,5,5	0.76	0	5,5,5	0.71	0
5	GOL	A	805	-	5,5,5	0.84	0	5,5,5	1.09	0
5	GOL	B	810	-	5,5,5	0.39	0	5,5,5	1.22	0
5	GOL	F	804	-	5,5,5	0.40	0	5,5,5	1.55	1 (20%)
5	GOL	C	806	-	5,5,5	0.25	0	5,5,5	0.89	0
6	PO4	B	812	-	4,4,4	0.87	0	6,6,6	0.54	0
5	GOL	A	813	-	5,5,5	0.67	0	5,5,5	1.09	1 (20%)
5	GOL	E	805	-	5,5,5	0.43	0	5,5,5	0.37	0
4	FOR	B	803	-	0,1,1	-	-	-		
5	GOL	A	809	-	5,5,5	0.88	0	5,5,5	0.69	0
5	GOL	D	705	-	5,5,5	0.43	0	5,5,5	0.15	0
5	GOL	B	809	-	5,5,5	1.03	0	5,5,5	0.63	0
5	GOL	A	811	-	5,5,5	0.46	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	B	811	-	5,5,5	0.40	0	5,5,5	1.02	0
5	GOL	D	704	-	5,5,5	0.32	0	5,5,5	0.99	0
5	GOL	F	812	-	5,5,5	0.73	0	5,5,5	1.00	0
4	FOR	A	803	-	0,1,1	-	-	-		
5	GOL	D	706	-	5,5,5	0.42	0	5,5,5	0.84	0
5	GOL	F	806	-	5,5,5	0.53	0	5,5,5	1.57	1 (20%)
5	GOL	F	803	-	5,5,5	0.61	0	5,5,5	0.72	0
5	GOL	D	712	-	5,5,5	0.98	0	5,5,5	1.03	0
5	GOL	C	810	-	5,5,5	0.59	0	5,5,5	0.69	0
5	GOL	B	806	-	5,5,5	0.39	0	5,5,5	0.50	0
3	PEO	E	802	2	1,1,1	0.89	0	-		
3	PEO	C	802	2	1,1,1	1.30	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
5	GOL	C	803	-	-	4/4/4/4	-
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	E	806	-	-	4/4/4/4	-
5	GOL	F	810	-	-	3/4/4/4	-
5	GOL	F	805	-	-	3/4/4/4	-
5	GOL	D	707	-	-	2/4/4/4	-
5	GOL	A	812	-	-	0/4/4/4	-
5	GOL	F	808	-	-	2/4/4/4	-
5	GOL	D	708	-	-	0/4/4/4	-
5	GOL	C	804	-	-	1/4/4/4	-
5	GOL	B	813	-	-	0/4/4/4	-
5	GOL	C	807	-	-	3/4/4/4	-
5	GOL	A	815	-	-	2/4/4/4	-
5	GOL	A	810	-	-	2/4/4/4	-
5	GOL	E	804	-	-	2/4/4/4	-
5	GOL	A	816	-	-	2/4/4/4	-
5	GOL	E	807	-	-	1/4/4/4	-
5	GOL	C	805	-	-	1/4/4/4	-
5	GOL	A	806	-	-	2/4/4/4	-
5	GOL	A	807	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	711	-	-	0/4/4/4	-
5	GOL	D	710	-	-	4/4/4/4	-
5	GOL	B	807	-	-	1/4/4/4	-
5	GOL	E	803	-	-	2/4/4/4	-
5	GOL	F	811	-	-	0/4/4/4	-
5	GOL	A	814	-	-	4/4/4/4	-
5	GOL	A	808	-	-	2/4/4/4	-
5	GOL	D	709	-	-	2/4/4/4	-
5	GOL	A	804	-	-	2/4/4/4	-
5	GOL	B	805	-	-	2/4/4/4	-
5	GOL	C	809	-	-	2/4/4/4	-
5	GOL	F	807	-	-	4/4/4/4	-
5	GOL	B	808	-	-	1/4/4/4	-
5	GOL	A	805	-	-	2/4/4/4	-
5	GOL	B	810	-	-	2/4/4/4	-
5	GOL	F	804	-	-	1/4/4/4	-
5	GOL	C	806	-	-	2/4/4/4	-
5	GOL	A	813	-	-	2/4/4/4	-
5	GOL	E	805	-	-	2/4/4/4	-
5	GOL	A	809	-	-	0/4/4/4	-
5	GOL	D	705	-	-	4/4/4/4	-
5	GOL	B	809	-	-	0/4/4/4	-
5	GOL	A	811	-	-	1/4/4/4	-
5	GOL	B	811	-	-	3/4/4/4	-
5	GOL	D	704	-	-	2/4/4/4	-
5	GOL	F	812	-	-	3/4/4/4	-
5	GOL	D	706	-	-	2/4/4/4	-
5	GOL	F	806	-	-	2/4/4/4	-
5	GOL	F	803	-	-	4/4/4/4	-
5	GOL	C	810	-	-	2/4/4/4	-
5	GOL	B	806	-	-	3/4/4/4	-
5	GOL	D	712	-	-	2/4/4/4	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	708	GOL	O1-C1-C2	-3.01	96.81	110.38
5	F	804	GOL	O3-C3-C2	-3.01	96.83	110.38
5	A	806	GOL	O3-C3-C2	-2.47	99.26	110.38
5	B	805	GOL	O2-C2-C1	-2.46	99.00	109.18
5	F	806	GOL	O2-C2-C1	-2.39	99.27	109.18

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	GOL	O1-C1-C2-C3
5	A	806	GOL	C1-C2-C3-O3
5	A	807	GOL	O1-C1-C2-C3
5	A	813	GOL	O1-C1-C2-C3
5	A	814	GOL	C1-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	FOR	1	0
5	A	816	GOL	1	0
5	D	711	GOL	5	0
5	A	804	GOL	1	0
5	B	805	GOL	2	0
5	A	805	GOL	1	0
5	A	813	GOL	2	0
5	E	805	GOL	3	0
5	D	705	GOL	1	0
5	D	704	GOL	1	0
5	F	812	GOL	1	0
4	A	803	FOR	1	0
5	D	712	GOL	2	0
5	C	810	GOL	2	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, 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	657/692 (94%)	-1.86	0	100	100	9, 19, 36, 77	5 (0%)
1	B	657/692 (94%)	-1.86	0	100	100	8, 19, 35, 84	4 (0%)
1	C	655/692 (94%)	-1.85	0	100	100	8, 19, 41, 75	10 (1%)
1	D	655/692 (94%)	-1.85	0	100	100	9, 20, 38, 86	9 (1%)
1	E	655/692 (94%)	-1.85	0	100	100	8, 20, 38, 87	5 (0%)
1	F	655/692 (94%)	-1.85	0	100	100	9, 19, 40, 75	7 (1%)
All	All	3934/4152 (94%)	-1.85	0	100	100	8, 19, 38, 87	40 (1%)

There are no RSRZ outliers to report.

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, 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	B-factors(Å^2)	Q<0.9
1	TYY	A	405	14/15	1.00	0.02	14,21,32,33	0
1	TYY	B	405	14/15	1.00	0.02	16,23,35,41	0
1	TYY	C	405	14/15	1.00	0.02	16,23,44,46	0
1	TYY	D	405	14/15	1.00	0.02	16,24,40,50	0
1	TYY	E	405	14/15	1.00	0.02	16,23,36,41	0
1	TYY	F	405	14/15	1.00	0.02	14,25,41,46	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
5	GOL	D	705	6/6	0.96	0.06	89,99,102,117	0
5	GOL	D	712	6/6	0.98	0.05	35,48,49,51	0
4	FOR	D	702	2/2	0.99	0.06	57,57,57,62	0
5	GOL	A	804	6/6	0.99	0.03	22,32,33,40	0
5	GOL	A	805	6/6	0.99	0.06	40,45,49,51	0
5	GOL	A	806	6/6	0.99	0.02	34,38,42,45	0
5	GOL	A	807	6/6	0.99	0.03	46,49,50,51	0
5	GOL	A	808	6/6	0.99	0.04	52,57,58,60	0
5	GOL	A	810	6/6	0.99	0.04	45,53,55,56	0
5	GOL	A	811	6/6	0.99	0.03	44,45,46,52	0
5	GOL	A	812	6/6	0.99	0.03	45,46,48,54	0
5	GOL	A	813	6/6	0.99	0.03	40,45,47,49	0
5	GOL	A	814	6/6	0.99	0.03	47,50,52,53	0
5	GOL	A	815	6/6	0.99	0.03	41,55,58,61	0
5	GOL	A	816	6/6	0.99	0.04	53,60,61,63	0
5	GOL	B	804	6/6	0.99	0.03	38,40,43,46	0
5	GOL	B	806	6/6	0.99	0.03	46,49,50,53	0
5	GOL	B	810	6/6	0.99	0.04	43,57,58,60	0
5	GOL	B	811	6/6	0.99	0.03	46,48,56,57	0
5	GOL	B	813	6/6	0.99	0.02	43,45,46,54	0
5	GOL	C	803	6/6	0.99	0.04	28,37,39,41	0
5	GOL	C	804	6/6	0.99	0.05	39,42,46,50	0
5	GOL	C	805	6/6	0.99	0.04	47,48,51,51	0
5	GOL	C	806	6/6	0.99	0.03	36,44,45,47	0
5	GOL	C	807	6/6	0.99	0.04	46,50,53,56	0
5	GOL	C	809	6/6	0.99	0.03	24,31,33,40	0
5	GOL	C	810	6/6	0.99	0.03	41,55,57,62	0
5	GOL	D	704	6/6	0.99	0.03	44,49,53,56	0
4	FOR	A	803	2/2	0.99	0.08	68,68,68,70	0
5	GOL	D	706	6/6	0.99	0.04	53,55,59,60	0
5	GOL	D	707	6/6	0.99	0.03	29,36,41,41	0
5	GOL	D	708	6/6	0.99	0.03	35,37,40,40	0
5	GOL	D	709	6/6	0.99	0.04	35,41,44,52	0
5	GOL	D	710	6/6	0.99	0.04	62,64,69,77	0
5	GOL	D	711	6/6	0.99	0.04	46,60,62,68	0
4	FOR	B	803	2/2	0.99	0.09	56,56,56,56	2
5	GOL	E	803	6/6	0.99	0.02	41,48,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	E	804	6/6	0.99	0.04	43,55,59,59	0
5	GOL	E	805	6/6	0.99	0.03	44,47,57,60	0
5	GOL	E	806	6/6	0.99	0.05	39,40,43,43	0
5	GOL	E	807	6/6	0.99	0.03	33,35,38,38	0
5	GOL	F	804	6/6	0.99	0.03	39,42,44,47	0
5	GOL	F	805	6/6	0.99	0.04	52,61,67,72	0
5	GOL	F	806	6/6	0.99	0.04	50,54,56,59	0
5	GOL	F	807	6/6	0.99	0.03	36,41,47,48	0
5	GOL	F	808	6/6	0.99	0.04	50,52,53,59	0
5	GOL	F	810	6/6	0.99	0.05	54,74,77,78	0
5	GOL	F	812	6/6	0.99	0.03	42,44,47,54	0
6	PO4	B	812	5/5	0.99	0.05	31,33,34,35	5
6	PO4	C	808	5/5	0.99	0.04	43,49,60,61	0
5	GOL	B	809	6/6	1.00	0.03	23,30,31,31	0
2	CU	F	801	1/1	1.00	0.01	19,19,19,19	0
3	PEO	A	802	2/2	1.00	0.01	14,14,14,20	0
3	PEO	B	802	2/2	1.00	0.03	13,13,13,21	0
5	GOL	A	809	6/6	1.00	0.04	23,28,29,30	0
3	PEO	C	802	2/2	1.00	0.01	14,14,14,17	0
3	PEO	D	701	2/2	1.00	0.01	17,17,17,17	0
3	PEO	E	802	2/2	1.00	0.03	14,14,14,20	0
5	GOL	F	803	6/6	1.00	0.03	30,34,38,39	0
3	PEO	F	802	2/2	1.00	0.01	13,13,13,16	0
2	CU	A	801	1/1	1.00	0.00	19,19,19,19	0
2	CU	B	801	1/1	1.00	0.00	20,20,20,20	0
2	CU	C	801	1/1	1.00	0.00	19,19,19,19	0
2	CU	D	703	1/1	1.00	0.01	20,20,20,20	0
5	GOL	B	805	6/6	1.00	0.03	35,52,59,60	0
5	GOL	F	811	6/6	1.00	0.04	24,27,29,30	0
2	CU	E	801	1/1	1.00	0.00	20,20,20,20	0
5	GOL	B	807	6/6	1.00	0.03	42,51,55,56	1
5	GOL	B	808	6/6	1.00	0.04	23,24,27,28	0
6	PO4	F	809	5/5	1.00	0.03	44,52,59,62	0

6.5 Other polymers (i)

There are no such residues in this entry.