Full wwPDB X-ray Structure Validation Report (i)

Jul 11, 2016 – 05:33 AM EDT

PDB ID	:	5F87
Title	:	Crystal structure of Drosophila Poglut1 (Rumi) complexed with UDP
Authors	:	Yu, H.J.; Li, H.L.
Deposited on	:	2015-12-09
Resolution	:	3.20 Å(reported)

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

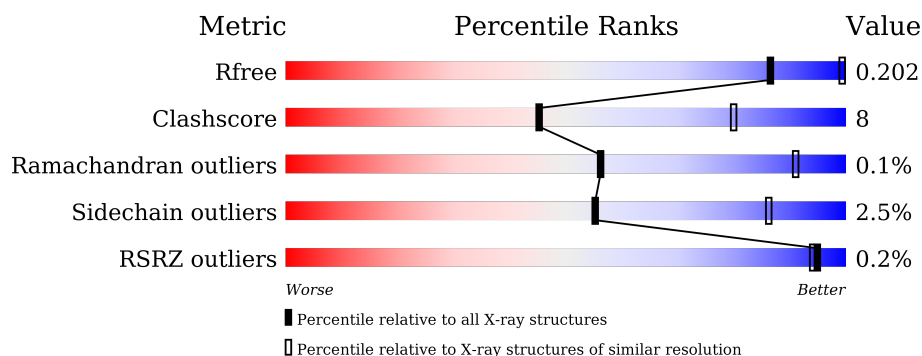|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 3.20 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	Percentile Ranks	Value
Rfree		0.202
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		2.5%
RSRZ outliers		0.2%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	402	73% 16% · 9%
1	B	402	77% 14% 9%
1	C	402	72% 17% · 9%
1	D	402	67% 23% 9%
1	E	402	71% 19% · 9%
1	F	402	72% 18% · 9%

WORLDWIDE PDB
PROTEIN DATA BANK

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	502	-	-	-	X
3	GOL	D	502	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18330 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 O-glucosyltransferase rumi.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			3024	1944	528	538	14			
1	B	365	Total	C	N	O	S	0	0	0
			3024	1944	528	538	14			
1	C	365	Total	C	N	O	S	0	0	0
			3024	1944	528	538	14			
1	D	365	Total	C	N	O	S	0	0	0
			3024	1944	528	538	14			
1	E	365	Total	C	N	O	S	0	0	0
			3024	1944	528	538	14			
1	F	365	Total	C	N	O	S	0	0	0
			3024	1944	528	538	14			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	-	expression tag	UNP Q8T045
A	14	ALA	-	expression tag	UNP Q8T045
A	15	GLN	-	expression tag	UNP Q8T045
A	16	PRO	-	expression tag	UNP Q8T045
A	17	ALA	-	expression tag	UNP Q8T045
A	18	GLU	-	expression tag	UNP Q8T045
A	19	ALA	-	expression tag	UNP Q8T045
A	20	LEU	-	expression tag	UNP Q8T045
A	408	ALA	-	expression tag	UNP Q8T045
A	409	ARG	-	expression tag	UNP Q8T045
A	410	ALA	-	expression tag	UNP Q8T045
A	411	LEU	-	expression tag	UNP Q8T045
A	412	VAL	-	expression tag	UNP Q8T045
A	413	PRO	-	expression tag	UNP Q8T045
A	414	ARG	-	expression tag	UNP Q8T045
B	13	ALA	-	expression tag	UNP Q8T045
B	14	ALA	-	expression tag	UNP Q8T045

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	GLN	-	expression tag	UNP Q8T045
B	16	PRO	-	expression tag	UNP Q8T045
B	17	ALA	-	expression tag	UNP Q8T045
B	18	GLU	-	expression tag	UNP Q8T045
B	19	ALA	-	expression tag	UNP Q8T045
B	20	LEU	-	expression tag	UNP Q8T045
B	408	ALA	-	expression tag	UNP Q8T045
B	409	ARG	-	expression tag	UNP Q8T045
B	410	ALA	-	expression tag	UNP Q8T045
B	411	LEU	-	expression tag	UNP Q8T045
B	412	VAL	-	expression tag	UNP Q8T045
B	413	PRO	-	expression tag	UNP Q8T045
B	414	ARG	-	expression tag	UNP Q8T045
C	13	ALA	-	expression tag	UNP Q8T045
C	14	ALA	-	expression tag	UNP Q8T045
C	15	GLN	-	expression tag	UNP Q8T045
C	16	PRO	-	expression tag	UNP Q8T045
C	17	ALA	-	expression tag	UNP Q8T045
C	18	GLU	-	expression tag	UNP Q8T045
C	19	ALA	-	expression tag	UNP Q8T045
C	20	LEU	-	expression tag	UNP Q8T045
C	408	ALA	-	expression tag	UNP Q8T045
C	409	ARG	-	expression tag	UNP Q8T045
C	410	ALA	-	expression tag	UNP Q8T045
C	411	LEU	-	expression tag	UNP Q8T045
C	412	VAL	-	expression tag	UNP Q8T045
C	413	PRO	-	expression tag	UNP Q8T045
C	414	ARG	-	expression tag	UNP Q8T045
D	13	ALA	-	expression tag	UNP Q8T045
D	14	ALA	-	expression tag	UNP Q8T045
D	15	GLN	-	expression tag	UNP Q8T045
D	16	PRO	-	expression tag	UNP Q8T045
D	17	ALA	-	expression tag	UNP Q8T045
D	18	GLU	-	expression tag	UNP Q8T045
D	19	ALA	-	expression tag	UNP Q8T045
D	20	LEU	-	expression tag	UNP Q8T045
D	408	ALA	-	expression tag	UNP Q8T045
D	409	ARG	-	expression tag	UNP Q8T045
D	410	ALA	-	expression tag	UNP Q8T045
D	411	LEU	-	expression tag	UNP Q8T045
D	412	VAL	-	expression tag	UNP Q8T045
D	413	PRO	-	expression tag	UNP Q8T045

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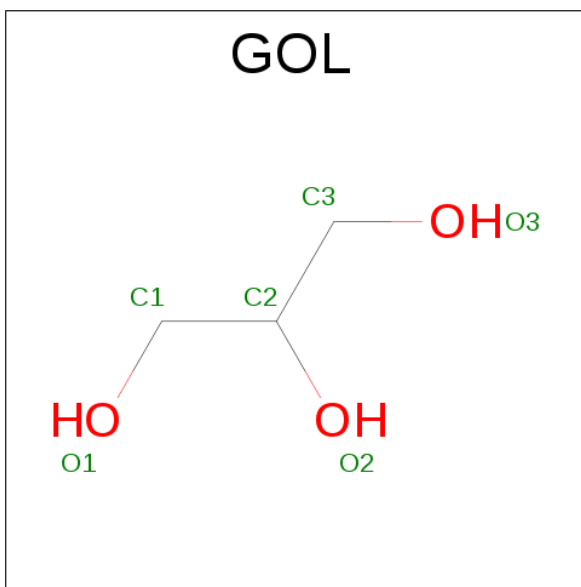
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Chain	Residue	Modelled	Actual	Comment	Reference
D	414	ARG	-	expression tag	UNP Q8T045
E	13	ALA	-	expression tag	UNP Q8T045
E	14	ALA	-	expression tag	UNP Q8T045
E	15	GLN	-	expression tag	UNP Q8T045
E	16	PRO	-	expression tag	UNP Q8T045
E	17	ALA	-	expression tag	UNP Q8T045
E	18	GLU	-	expression tag	UNP Q8T045
E	19	ALA	-	expression tag	UNP Q8T045
E	20	LEU	-	expression tag	UNP Q8T045
E	408	ALA	-	expression tag	UNP Q8T045
E	409	ARG	-	expression tag	UNP Q8T045
E	410	ALA	-	expression tag	UNP Q8T045
E	411	LEU	-	expression tag	UNP Q8T045
E	412	VAL	-	expression tag	UNP Q8T045
E	413	PRO	-	expression tag	UNP Q8T045
E	414	ARG	-	expression tag	UNP Q8T045
F	13	ALA	-	expression tag	UNP Q8T045
F	14	ALA	-	expression tag	UNP Q8T045
F	15	GLN	-	expression tag	UNP Q8T045
F	16	PRO	-	expression tag	UNP Q8T045
F	17	ALA	-	expression tag	UNP Q8T045
F	18	GLU	-	expression tag	UNP Q8T045
F	19	ALA	-	expression tag	UNP Q8T045
F	20	LEU	-	expression tag	UNP Q8T045
F	408	ALA	-	expression tag	UNP Q8T045
F	409	ARG	-	expression tag	UNP Q8T045
F	410	ALA	-	expression tag	UNP Q8T045
F	411	LEU	-	expression tag	UNP Q8T045
F	412	VAL	-	expression tag	UNP Q8T045
F	413	PRO	-	expression tag	UNP Q8T045
F	414	ARG	-	expression tag	UNP Q8T045

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).
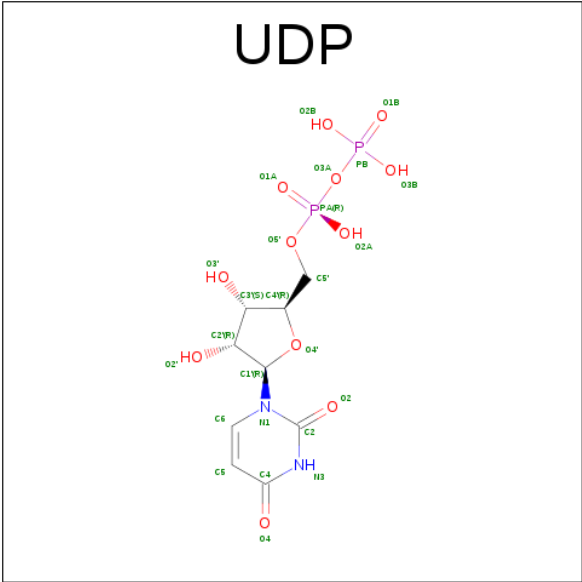
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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

GOL

C3

OH O3

C1   C2

HO

O1

OH

O2

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

3 Residue-property plots ⓘ

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

- Molecule 1: O-glucosyltransferase rumi
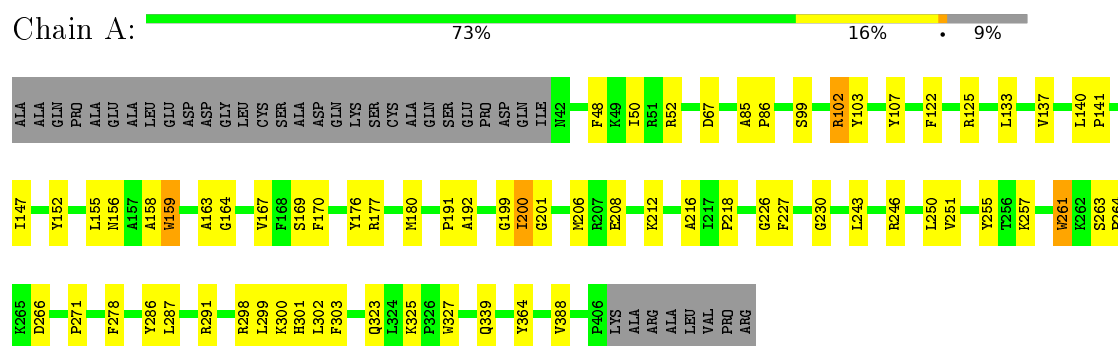
Chain A:

- Molecule 1: O-glucosyltransferase rumi
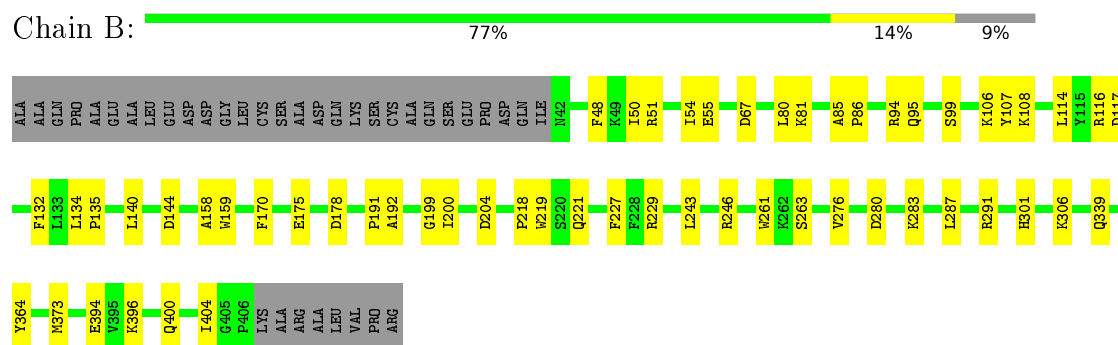
Chain B:

- Molecule 1: O-glucosyltransferase rumi

Chain C:
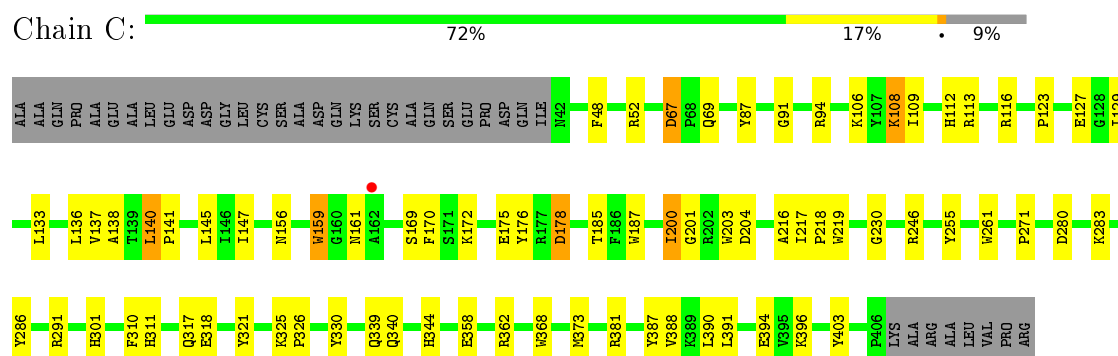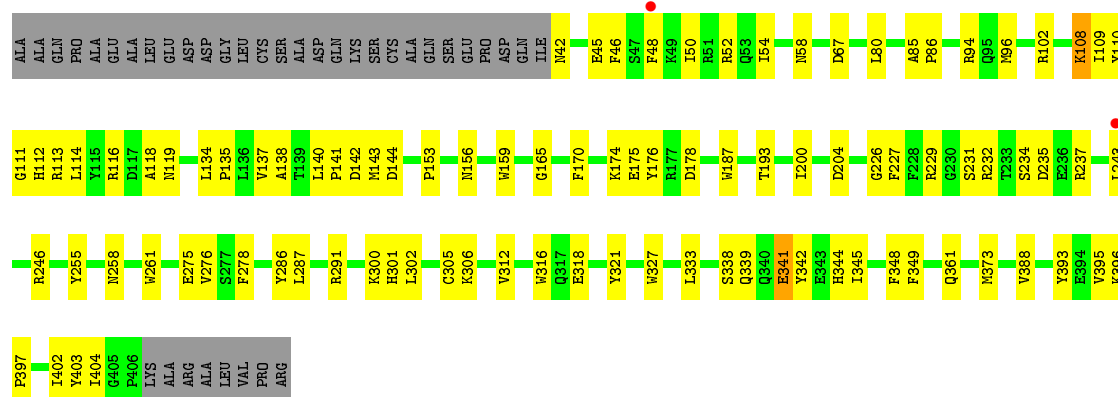
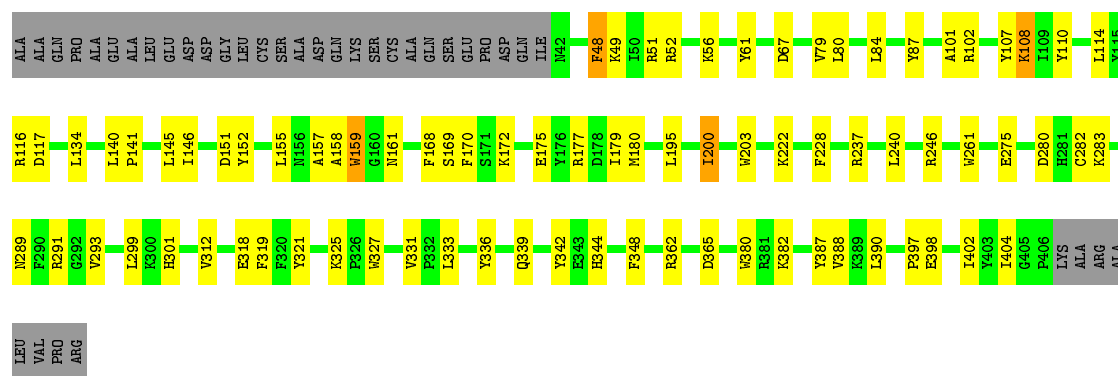• Molecule 1: O-glucosyltransferase rumi

Chain D:
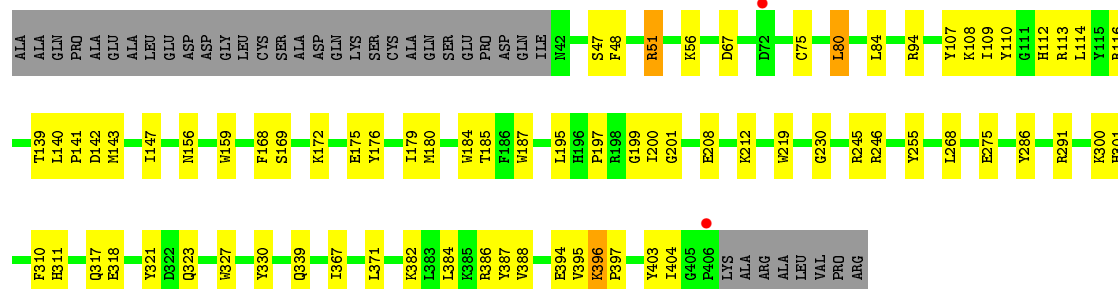

• Molecule 1: O-glucosyltransferase rumi

Chain E:

• Molecule 1: O-glucosyltransferase rumi

Chain F:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	241.91Å 241.91Å 47.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 35.11 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-3.20) 98.6 (35.11-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.168 , 0.203 0.169 , 0.202	Depositor DCC
R_{free} test set	2539 reflections (5.34%)	DCC
Wilson B-factor (Å²)	40.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.37 , 10.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.137 for -h,-k,l 0.137 for h,-h-k,-l 0.458 for -k,-h,-l	Xtriage
Reported twinning fraction	0.496 for H, K, L 0.504 for -K, -H, -L	Depositor
Outliers	0 of 50131 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	18330	wwPDB-VP
Average B, all atoms (Å²)	34.0	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UDP

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	0.57	2/3114 (0.1%)	0.61	0/4208
1	B	0.57	2/3114 (0.1%)	0.60	0/4208
1	C	0.58	5/3114 (0.2%)	0.61	0/4208
1	D	0.59	5/3114 (0.2%)	0.62	1/4208 (0.0%)
1	E	0.58	3/3114 (0.1%)	0.63	0/4208
1	F	0.59	5/3114 (0.2%)	0.62	0/4208
All	All	0.58	22/18684 (0.1%)	0.62	1/25248 (0.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	261	TRP	CD2-CE2	5.75	1.48	1.41
1	C	368	TRP	CD2-CE2	5.32	1.47	1.41
1	B	219	TRP	CD2-CE2	5.25	1.47	1.41
1	E	380	TRP	CD2-CE2	5.22	1.47	1.41
1	C	203	TRP	CD2-CE2	5.22	1.47	1.41
1	C	187	TRP	CD2-CE2	5.21	1.47	1.41
1	A	261	TRP	CD2-CE2	5.20	1.47	1.41
1	A	159	TRP	CD2-CE2	5.19	1.47	1.41
1	D	159	TRP	CD2-CE2	5.18	1.47	1.41
1	D	261	TRP	CD2-CE2	5.16	1.47	1.41
1	C	261	TRP	CD2-CE2	5.14	1.47	1.41
1	B	261	TRP	CD2-CE2	5.14	1.47	1.41
1	F	187	TRP	CD2-CE2	5.14	1.47	1.41
1	E	203	TRP	CD2-CE2	5.10	1.47	1.41
1	F	159	TRP	CD2-CE2	5.09	1.47	1.41
1	C	219	TRP	CD2-CE2	5.09	1.47	1.41
1	F	219	TRP	CD2-CE2	5.09	1.47	1.41
1	F	327	TRP	CD2-CE2	5.08	1.47	1.41
1	D	187	TRP	CD2-CE2	5.05	1.47	1.41
1	D	327	TRP	CD2-CE2	5.03	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	184	TRP	CD2-CE2	5.01	1.47	1.41
1	D	316	TRP	CD2-CE2	5.00	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	80	LEU	CA-CB-CG	5.20	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	2936	54	0
1	B	3024	0	2936	37	0
1	C	3024	0	2936	44	0
1	D	3024	0	2936	82	1
1	E	3024	0	2936	53	1
1	F	3024	0	2936	42	0
2	A	25	0	11	2	0
2	B	25	0	11	1	0
2	C	25	0	11	0	0
2	D	25	0	11	1	0
2	E	25	0	11	1	0
2	F	25	0	11	0	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
All	All	18330	0	17730	282	1

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 8.

All (282) 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:84:LEU:HD12	1:F:386:ARG:HD3	1.38	1.02
1:D:113:ARG:HD3	1:D:403:TYR:HE1	1.35	0.92
1:D:113:ARG:HD3	1:D:403:TYR:CE1	2.10	0.87
1:C:246:ARG:HE	1:C:339:GLN:HE22	1.27	0.81
1:D:46:PHE:CZ	1:D:344:HIS:HB3	2.22	0.74
1:D:144:ASP:HB2	1:D:393:TYR:OH	1.87	0.74
1:A:271:PRO:HA	1:D:402:ILE:HD12	1.70	0.73
1:C:113:ARG:HD3	1:C:403:TYR:HE1	1.50	0.73
1:C:113:ARG:HD3	1:C:403:TYR:CE1	2.25	0.72
1:D:174:LYS:HB3	1:E:52:ARG:HH21	1.54	0.72
1:A:246:ARG:HH21	1:A:339:GLN:HE21	1.35	0.70
1:F:396:LYS:HB2	1:F:396:LYS:NZ	2.06	0.70
1:D:48:PHE:CD1	1:E:158:ALA:HB2	2.27	0.69
1:F:318:GLU:HB2	1:F:321:TYR:CE1	2.27	0.69
1:D:116:ARG:HB3	1:D:404:ILE:HD11	1.75	0.69
1:C:138:ALA:O	1:F:110:TYR:OH	2.11	0.69
1:A:206:MET:HG2	1:A:301:HIS:CD2	2.28	0.69
1:E:169:SER:O	1:E:180:MET:HA	1.93	0.69
1:F:107:TYR:HD1	1:F:114:LEU:HD11	1.58	0.68
1:A:48:PHE:CE2	1:B:175:GLU:HB2	2.28	0.68
1:A:158:ALA:HB2	1:B:48:PHE:HE1	1.59	0.68
1:B:246:ARG:HH21	1:B:339:GLN:HE21	1.43	0.66
1:A:246:ARG:HE	1:A:339:GLN:HE22	1.44	0.66
1:A:271:PRO:HG3	1:D:404:ILE:HA	1.77	0.66
1:D:174:LYS:HB3	1:E:52:ARG:NH2	2.11	0.65
1:C:172:LYS:HD3	1:C:178:ASP:O	1.95	0.65
1:D:85:ALA:HB3	1:D:86:PRO:HD3	1.77	0.65
1:B:246:ARG:HH21	1:B:339:GLN:NE2	1.95	0.65
1:D:48:PHE:CE2	1:D:52:ARG:HD2	2.33	0.64
1:D:94:ARG:HB2	1:D:94:ARG:NH1	2.13	0.63
1:C:87:TYR:HB2	1:C:390:LEU:HD13	1.79	0.62
1:A:263:SER:HB2	1:A:264:PRO:HD2	1.82	0.62
1:D:193:THR:HB	1:D:275:GLU:OE1	1.99	0.62
1:E:141:PRO:HG2	1:E:388:VAL:HG11	1.81	0.62
1:D:204:ASP:HB3	1:D:373:MET:HG3	1.82	0.61
1:F:141:PRO:HG2	1:F:388:VAL:HG11	1.82	0.61
1:A:299:LEU:HG	1:A:303:PHE:HE2	1.65	0.61
1:B:94:ARG:NH2	1:B:394:GLU:O	2.33	0.61
1:F:80:LEU:O	1:F:84:LEU:HG	2.01	0.61
1:F:246:ARG:HH21	1:F:339:GLN:NE2	1.99	0.61

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:O	1:B:55:GLU:HG3	2.01	0.60
1:D:141:PRO:HG2	1:D:388:VAL:HG21	1.84	0.60
1:C:246:ARG:HH21	1:C:339:GLN:HE21	1.49	0.60
1:D:235:ASP:OD2	1:E:344:HIS:NE2	2.34	0.60
1:D:110:TYR:CZ	1:D:397:PRO:HD3	2.37	0.59
1:C:216:ALA:O	1:C:218:PRO:HD3	2.02	0.59
1:E:107:TYR:HD1	1:E:114:LEU:HD11	1.67	0.59
1:E:101:ALA:HA	1:E:146:ILE:HD12	1.82	0.59
1:D:338:SER:HB3	1:E:336:TYR:O	2.03	0.58
1:C:246:ARG:HE	1:C:339:GLN:NE2	2.00	0.58
1:F:109:ILE:O	1:F:142:ASP:HA	2.03	0.58
1:F:200:ILE:HD11	1:F:301:HIS:NE2	2.19	0.58
1:D:275:GLU:HG3	2:D:501:UDP:C4	2.40	0.57
1:E:87:TYR:HB2	1:E:390:LEU:HD13	1.87	0.57
1:D:94:ARG:HB2	1:D:94:ARG:HH11	1.70	0.57
1:C:388:VAL:HA	1:C:391:LEU:HD13	1.87	0.57
1:E:200:ILE:HD11	1:E:301:HIS:CE1	2.40	0.56
1:B:132:PHE:O	1:B:135:PRO:HD2	2.05	0.56
1:C:109:ILE:HG23	1:C:137:VAL:HG13	1.88	0.56
1:D:50:ILE:HG22	1:D:54:ILE:HD11	1.86	0.56
1:D:45:GLU:HG2	1:E:152:TYR:OH	2.05	0.56
1:E:246:ARG:HE	1:E:339:GLN:HE22	1.54	0.56
1:B:50:ILE:HG22	1:B:54:ILE:HD11	1.88	0.55
1:A:246:ARG:HE	1:A:339:GLN:NE2	2.03	0.55
1:C:141:PRO:HG2	1:C:388:VAL:HG11	1.87	0.55
1:C:133:LEU:O	1:C:137:VAL:HG23	2.07	0.55
1:D:338:SER:OG	1:E:336:TYR:HB3	2.07	0.55
1:E:289:ASN:ND2	1:E:299:LEU:HB2	2.22	0.54
1:D:111:GLY:H	1:D:142:ASP:CG	2.11	0.54
1:C:394:GLU:CD	1:F:139:THR:HB	2.28	0.54
1:F:107:TYR:CD2	1:F:147:ILE:HD12	2.43	0.54
1:D:156:ASN:ND2	1:D:175:GLU:OE2	2.41	0.54
1:D:246:ARG:HE	1:D:339:GLN:NE2	2.06	0.54
1:D:231:SER:HB2	1:D:258:ASN:HD22	1.72	0.54
1:C:123:PRO:O	1:C:127:GLU:HG3	2.07	0.54
1:D:237:ARG:HB2	1:D:255:TYR:OH	2.07	0.54
1:F:286:TYR:HB3	1:F:310:PHE:CE1	2.44	0.53
1:D:338:SER:O	1:D:341:GLU:HB3	2.08	0.53
1:A:48:PHE:CD2	1:A:48:PHE:C	2.81	0.53
1:C:185:THR:O	1:C:201:GLY:HA2	2.08	0.53
1:E:280:ASP:O	1:E:283:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:TYR:HA	1:D:142:ASP:CG	2.29	0.53
1:D:42:ASN:O	1:D:45:GLU:HB2	2.08	0.53
1:C:94:ARG:NH2	1:C:394:GLU:O	2.41	0.53
1:A:216:ALA:O	1:A:218:PRO:HD3	2.08	0.53
1:B:107:TYR:HD1	1:B:114:LEU:HD11	1.74	0.53
1:B:134:LEU:HD21	1:B:404:ILE:HG22	1.91	0.52
1:D:112:HIS:CE1	1:D:140:LEU:O	2.61	0.52
1:D:318:GLU:HB2	1:D:321:TYR:CE1	2.44	0.52
1:C:112:HIS:CE1	1:C:140:LEU:O	2.62	0.52
1:C:87:TYR:O	1:C:91:GLY:N	2.41	0.52
1:E:110:TYR:CZ	1:E:397:PRO:HD3	2.45	0.52
1:E:228:PHE:CZ	1:E:237:ARG:HD3	2.44	0.52
1:A:141:PRO:HG2	1:A:388:VAL:HG21	1.90	0.52
1:C:286:TYR:HB3	1:C:310:PHE:CE1	2.45	0.52
1:B:108:LYS:HE2	1:B:396:LYS:O	2.11	0.51
1:F:195:LEU:HB2	1:F:275:GLU:OE2	2.10	0.51
1:D:48:PHE:CE2	1:E:175:GLU:HA	2.46	0.51
1:D:175:GLU:CD	1:E:48:PHE:CZ	2.83	0.51
1:D:48:PHE:HD1	1:E:158:ALA:HB2	1.74	0.51
1:D:108:LYS:HE2	1:D:396:LYS:O	2.10	0.51
1:A:48:PHE:HE1	1:B:158:ALA:HB2	1.76	0.51
1:D:50:ILE:O	1:D:54:ILE:HG13	2.10	0.51
1:F:47:SER:O	1:F:51:ARG:HD3	2.11	0.51
1:F:311:HIS:HB3	1:F:330:TYR:CD2	2.46	0.50
1:D:144:ASP:HB2	1:D:393:TYR:HH	1.76	0.50
1:D:110:TYR:CE1	1:D:397:PRO:HD3	2.47	0.50
1:C:67:ASP:OD1	1:C:69:GLN:HB2	2.12	0.50
1:A:271:PRO:HA	1:D:402:ILE:CD1	2.41	0.50
1:C:145:LEU:HD23	1:C:387:TYR:CE1	2.47	0.50
1:F:245:ARG:HH22	1:F:268:LEU:HB2	1.76	0.50
1:B:218:PRO:HD2	1:B:221:GLN:OE1	2.11	0.49
1:F:311:HIS:HB3	1:F:330:TYR:CE2	2.47	0.49
1:D:46:PHE:CE1	1:D:344:HIS:HB3	2.46	0.49
1:F:110:TYR:CZ	1:F:397:PRO:HD3	2.46	0.49
1:A:257:LYS:NZ	1:D:119:ASN:HA	2.27	0.49
1:D:246:ARG:HE	1:D:339:GLN:HE22	1.60	0.49
1:F:112:HIS:O	1:F:113:ARG:HG2	2.13	0.49
1:A:300:LYS:HE2	1:A:301:HIS:CE1	2.48	0.49
1:B:364:TYR:C	1:B:364:TYR:CD1	2.86	0.49
1:B:48:PHE:C	1:B:48:PHE:CD2	2.85	0.49
1:B:80:LEU:HD12	1:B:81:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:GLU:HB2	1:E:321:TYR:CE1	2.48	0.49
1:B:306:LYS:HG3	1:B:364:TYR:CD2	2.48	0.49
1:F:367:ILE:HD12	1:F:371:LEU:HD22	1.94	0.49
1:A:191:PRO:HG2	2:A:501:UDP:H4'	1.95	0.49
1:A:48:PHE:CE1	1:B:158:ALA:HB2	2.48	0.49
1:B:227:PHE:HB3	1:B:287:LEU:HD23	1.95	0.49
1:B:404:ILE:HD13	1:C:271:PRO:HG3	1.95	0.49
1:F:108:LYS:HD3	1:F:110:TYR:HB2	1.94	0.49
1:F:396:LYS:HB2	1:F:396:LYS:HZ2	1.76	0.49
1:A:155:LEU:HD22	1:A:163:ALA:HA	1.95	0.48
1:D:338:SER:CB	1:E:336:TYR:O	2.62	0.48
1:C:204:ASP:HB3	1:C:373:MET:HG3	1.94	0.48
1:D:243:LEU:HD13	1:D:339:GLN:HB3	1.96	0.48
1:B:108:LYS:NZ	1:B:144:ASP:OD1	2.32	0.47
1:D:300:LYS:HE2	1:D:301:HIS:CE1	2.49	0.47
1:D:54:ILE:O	1:D:58:ASN:ND2	2.33	0.47
1:A:250:LEU:HG	1:A:251:VAL:HG23	1.96	0.47
1:D:227:PHE:HB3	1:D:287:LEU:HD23	1.96	0.47
1:F:116:ARG:HB3	1:F:404:ILE:HD11	1.96	0.47
1:A:192:ALA:HA	1:A:199:GLY:HA2	1.95	0.47
1:B:280:ASP:O	1:B:283:LYS:HG2	2.14	0.47
1:D:109:ILE:HG12	1:D:137:VAL:HG22	1.97	0.47
1:F:75:CYS:O	1:F:323:GLN:HG3	2.14	0.47
1:C:159:TRP:N	1:C:159:TRP:CD1	2.82	0.47
1:F:80:LEU:HD21	1:F:382:LYS:HG2	1.96	0.47
1:D:143:MET:HA	1:D:395:VAL:HG21	1.97	0.47
1:C:176:TYR:HB3	1:C:178:ASP:OD1	2.14	0.47
1:A:271:PRO:CA	1:D:402:ILE:HD12	2.42	0.47
1:E:159:TRP:CD1	1:E:159:TRP:N	2.83	0.47
1:D:226:GLY:HA2	1:D:286:TYR:HB2	1.97	0.47
1:A:133:LEU:O	1:A:137:VAL:HG23	2.15	0.46
1:C:317:GLN:HA	1:C:321:TYR:CD2	2.50	0.46
1:B:229:ARG:HG2	1:B:276:VAL:HG23	1.96	0.46
1:D:134:LEU:HB2	1:D:135:PRO:HD3	1.98	0.46
1:B:106:LYS:O	1:B:116:ARG:HA	2.15	0.46
1:C:200:ILE:HD11	1:C:301:HIS:CE1	2.51	0.46
1:E:362:ARG:HA	1:E:365:ASP:HB2	1.98	0.46
1:A:48:PHE:CG	1:B:175:GLU:OE2	2.68	0.46
1:D:46:PHE:O	1:D:50:ILE:HG12	2.16	0.46
1:E:222:LYS:NZ	1:E:282:CYS:O	2.48	0.46
1:E:246:ARG:HH21	1:E:339:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:PHE:CE2	1:D:344:HIS:HB3	2.50	0.45
1:C:358:GLU:O	1:C:362:ARG:HG3	2.15	0.45
1:D:110:TYR:CD1	1:D:142:ASP:OD2	2.69	0.45
1:E:168:PHE:HA	1:E:179:ILE:O	2.17	0.45
1:A:156:ASN:HB3	1:A:159:TRP:CD2	2.51	0.45
1:B:50:ILE:O	1:B:54:ILE:HG13	2.16	0.45
1:B:85:ALA:HB3	1:B:86:PRO:HD3	1.97	0.45
1:D:306:LYS:HE2	1:D:361:GLN:OE1	2.17	0.45
1:B:95:GLN:HE21	1:B:99:SER:HB2	1.81	0.45
1:D:302:LEU:O	1:D:305:CYS:HB2	2.17	0.45
1:E:116:ARG:HG2	1:E:117:ASP:N	2.32	0.45
1:F:113:ARG:HD3	1:F:403:TYR:HE1	1.82	0.45
1:A:323:GLN:HA	1:A:325:LYS:HE2	1.99	0.45
1:F:94:ARG:NH2	1:F:394:GLU:O	2.50	0.45
1:A:226:GLY:HA2	1:A:286:TYR:HB2	1.97	0.44
1:E:246:ARG:HH21	1:E:339:GLN:NE2	2.14	0.44
1:C:106:LYS:O	1:C:116:ARG:HA	2.18	0.44
1:D:229:ARG:HG2	1:D:276:VAL:HG23	1.98	0.44
1:F:197:PRO:C	1:F:199:GLY:H	2.20	0.44
1:A:200:ILE:HG12	1:A:201:GLY:N	2.33	0.44
1:D:153:PRO:HB2	1:D:176:TYR:CD1	2.53	0.44
1:C:325:LYS:HA	1:C:326:PRO:HD2	1.77	0.44
1:E:348:PHE:C	1:E:348:PHE:CD2	2.91	0.44
1:F:208:GLU:O	1:F:212:LYS:HD3	2.18	0.44
1:A:200:ILE:HD12	1:A:278:PHE:CE2	2.53	0.44
1:C:318:GLU:HB2	1:C:321:TYR:CE1	2.53	0.44
1:A:107:TYR:CD2	1:A:147:ILE:HD12	2.53	0.44
1:A:169:SER:O	1:A:180:MET:HA	2.18	0.44
1:A:50:ILE:HG23	1:A:327:TRP:CZ3	2.53	0.44
1:A:99:SER:O	1:A:102:ARG:HG2	2.18	0.44
1:E:327:TRP:CZ3	1:E:331:VAL:HG13	2.52	0.44
1:E:155:LEU:HB3	1:E:177:ARG:HB2	2.00	0.43
1:A:48:PHE:CZ	1:A:52:ARG:HB2	2.54	0.43
1:C:108:LYS:CE	1:C:396:LYS:O	2.66	0.43
1:E:157:ALA:HA	1:E:177:ARG:NH1	2.33	0.43
1:F:185:THR:O	1:F:201:GLY:HA2	2.18	0.43
1:A:164:GLY:HA2	1:A:177:ARG:HE	1.82	0.43
1:D:342:TYR:O	1:D:345:ILE:HG22	2.17	0.43
1:B:192:ALA:HA	1:B:199:GLY:HA2	2.01	0.43
1:F:300:LYS:HE2	1:F:301:HIS:CE1	2.52	0.43
1:E:237:ARG:HH22	2:E:501:UDP:PB	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:GLN:HE21	1:E:339:GLN:HB3	1.52	0.43
1:C:136:LEU:HD22	1:C:381:ARG:HG3	2.01	0.43
1:D:200:ILE:HD12	1:D:278:PHE:CE2	2.54	0.43
1:E:108:LYS:NZ	1:E:398:GLU:OE1	2.46	0.43
1:A:261:TRP:CD1	1:A:266:ASP:HB2	2.54	0.43
2:A:501:UDP:O2B	3:A:502:GOL:O1	2.21	0.43
1:C:217:ILE:HD13	1:C:283:LYS:HB3	2.01	0.43
1:D:232:ARG:HD2	1:D:255:TYR:CE2	2.54	0.43
1:D:345:ILE:O	1:D:349:PHE:HD2	2.02	0.43
1:E:240:LEU:HB2	1:E:342:TYR:CZ	2.54	0.43
1:E:79:VAL:HG21	1:E:319:PHE:O	2.18	0.43
1:A:364:TYR:CD1	1:A:364:TYR:C	2.92	0.42
1:F:230:GLY:O	1:F:255:TYR:HA	2.17	0.42
1:F:367:ILE:HA	1:F:367:ILE:HD13	1.91	0.42
1:B:200:ILE:HD11	1:B:301:HIS:CE1	2.53	0.42
1:A:122:PHE:CB	1:A:125:ARG:HD2	2.49	0.42
1:A:152:TYR:HE2	1:A:176:TYR:HH	1.66	0.42
1:B:191:PRO:HG2	2:B:501:UDP:H4'	2.01	0.42
1:C:246:ARG:HH21	1:C:339:GLN:NE2	2.15	0.42
1:D:108:LYS:HE3	1:D:395:VAL:HG12	2.00	0.42
1:F:168:PHE:HA	1:F:179:ILE:O	2.19	0.42
1:F:169:SER:O	1:F:180:MET:HA	2.19	0.42
1:A:226:GLY:HA2	1:A:286:TYR:O	2.18	0.42
1:A:261:TRP:HZ2	1:D:118:ALA:HB1	1.85	0.42
1:D:48:PHE:CD2	1:E:175:GLU:HG3	2.55	0.42
1:C:129:ILE:HD13	1:C:147:ILE:HG21	2.01	0.42
1:F:156:ASN:ND2	1:F:175:GLU:OE2	2.53	0.42
1:C:311:HIS:HB3	1:C:330:TYR:CD2	2.54	0.42
1:A:287:LEU:HD13	1:A:302:LEU:HD22	2.01	0.42
1:D:312:VAL:HG22	1:D:333:LEU:HB2	2.02	0.42
1:E:80:LEU:HD21	1:E:382:LYS:HG2	2.01	0.42
1:D:111:GLY:N	1:D:142:ASP:OD1	2.46	0.42
1:E:48:PHE:HA	1:E:51:ARG:NH1	2.35	0.42
1:A:243:LEU:HB2	1:A:339:GLN:HG2	2.02	0.42
1:A:85:ALA:HB3	1:A:86:PRO:HD3	2.02	0.41
1:D:48:PHE:CE1	1:E:158:ALA:HB2	2.54	0.41
1:E:312:VAL:HG22	1:E:333:LEU:HD12	2.02	0.41
1:F:172:LYS:HB2	1:F:176:TYR:HB2	2.01	0.41
1:F:384:LEU:O	1:F:387:TYR:HB3	2.20	0.41
1:C:230:GLY:O	1:C:255:TYR:HA	2.20	0.41
1:E:145:LEU:HD23	1:E:387:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:PHE:CD2	1:E:49:LYS:N	2.88	0.41
1:B:116:ARG:HG2	1:B:117:ASP:N	2.35	0.41
1:D:46:PHE:CZ	1:D:344:HIS:CB	2.99	0.41
1:D:94:ARG:CB	1:D:94:ARG:HH11	2.34	0.41
1:D:94:ARG:HH12	1:D:393:TYR:HB2	1.84	0.41
1:E:195:LEU:HB2	1:E:275:GLU:OE2	2.20	0.41
1:A:230:GLY:O	1:A:255:TYR:HA	2.20	0.41
1:C:156:ASN:ND2	1:C:175:GLU:OE2	2.54	0.41
1:D:96:MET:HB3	1:D:165:GLY:O	2.20	0.41
1:B:400:GLN:OE1	1:B:400:GLN:N	2.52	0.41
1:D:234:SER:O	1:D:237:ARG:HG3	2.19	0.41
1:E:134:LEU:HD21	1:E:404:ILE:HG22	2.03	0.41
1:C:340:GLN:O	1:C:344:HIS:ND1	2.53	0.41
1:A:48:PHE:CZ	1:A:52:ARG:HD2	2.56	0.41
1:D:338:SER:HG	1:E:336:TYR:HB3	1.86	0.41
1:F:394:GLU:O	1:F:396:LYS:HG3	2.21	0.41
1:A:208:GLU:O	1:A:212:LYS:HG3	2.21	0.41
1:C:48:PHE:CE2	1:C:52:ARG:HD2	2.56	0.41
1:D:50:ILE:HG21	1:D:348:PHE:CE2	2.56	0.41
1:E:151:ASP:HB2	1:E:293:VAL:HG11	2.02	0.41
1:F:317:GLN:HA	1:F:321:TYR:CD2	2.56	0.41
1:A:227:PHE:N	1:A:286:TYR:O	2.48	0.41
1:B:204:ASP:HB3	1:B:373:MET:HG3	2.02	0.41
1:E:84:LEU:HB3	1:E:390:LEU:HD11	2.03	0.41
1:A:103:TYR:HB2	1:A:167:VAL:HG21	2.02	0.40
1:F:143:MET:HA	1:F:395:VAL:HG21	2.03	0.40
1:A:246:ARG:HH21	1:A:339:GLN:NE2	2.11	0.40
1:B:243:LEU:HD13	1:B:339:GLN:HB3	2.02	0.40
1:D:344:HIS:CE1	1:E:336:TYR:CZ	3.09	0.40
1:A:298:ARG:HG2	1:A:302:LEU:HG	2.02	0.40
1:E:61:TYR:CE2	1:E:325:LYS:HG3	2.57	0.40
1:B:276:VAL:CG1	1:B:280:ASP:HB2	2.52	0.40
1:C:280:ASP:O	1:C:283:LYS:HG2	2.22	0.40
1:D:114:LEU:HB3	1:D:404:ILE:HB	2.03	0.40
1:A:48:PHE:CE2	1:B:175:GLU:CB	3.02	0.40
1:C:169:SER:HB2	1:C:178:ASP:HB3	2.04	0.40
1:A:261:TRP:CZ3	1:D:119:ASN:HB2	2.56	0.40

All (1) 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:D:138:ALA:O	1:E:110:TYR:OH[3_564]	2.06	0.14

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	363/402 (90%)	350 (96%)	13 (4%)	0	100	100
1	B	363/402 (90%)	350 (96%)	13 (4%)	0	100	100
1	C	363/402 (90%)	351 (97%)	11 (3%)	1 (0%)	46	85
1	D	363/402 (90%)	348 (96%)	15 (4%)	0	100	100
1	E	363/402 (90%)	350 (96%)	12 (3%)	1 (0%)	46	85
1	F	363/402 (90%)	344 (95%)	19 (5%)	0	100	100
All	All	2178/2412 (90%)	2093 (96%)	83 (4%)	2 (0%)	56	91

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	ASN
1	E	161	ASN

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	318/348 (91%)	312 (98%)	6 (2%)	65	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	318/348 (91%)	311 (98%)	7 (2%)	60	87
1	C	318/348 (91%)	310 (98%)	8 (2%)	55	86
1	D	318/348 (91%)	311 (98%)	7 (2%)	60	87
1	E	318/348 (91%)	306 (96%)	12 (4%)	40	78
1	F	318/348 (91%)	310 (98%)	8 (2%)	55	86
All	All	1908/2088 (91%)	1860 (98%)	48 (2%)	55	86

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	102	ARG
1	A	140	LEU
1	A	170	PHE
1	A	200	ILE
1	A	291	ARG
1	B	67	ASP
1	B	140	LEU
1	B	159	TRP
1	B	170	PHE
1	B	178	ASP
1	B	263	SER
1	B	291	ARG
1	C	67	ASP
1	C	108	LYS
1	C	140	LEU
1	C	159	TRP
1	C	170	PHE
1	C	178	ASP
1	C	200	ILE
1	C	291	ARG
1	D	67	ASP
1	D	102	ARG
1	D	108	LYS
1	D	170	PHE
1	D	178	ASP
1	D	291	ARG
1	D	341	GLU
1	E	48	PHE
1	E	56	LYS

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Mol	Chain	Res	Type
1	E	67	ASP
1	E	102	ARG
1	E	108	LYS
1	E	140	LEU
1	E	159	TRP
1	E	170	PHE
1	E	172	LYS
1	E	200	ILE
1	E	291	ARG
1	E	402	ILE
1	F	48	PHE
1	F	51	ARG
1	F	56	LYS
1	F	67	ASP
1	F	80	LEU
1	F	140	LEU
1	F	291	ARG
1	F	396	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	301	HIS
1	A	339	GLN
1	B	95	GLN
1	B	339	GLN
1	C	95	GLN
1	C	154	GLN
1	C	254	GLN
1	C	301	HIS
1	C	329	HIS
1	C	339	GLN
1	C	361	GLN
1	D	95	GLN
1	D	339	GLN
1	E	95	GLN
1	E	254	GLN
1	E	289	ASN
1	E	301	HIS
1	E	339	GLN
1	F	95	GLN

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Mol	Chain	Res	Type
1	F	339	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 ligands 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	#$|Z| > 2$
2	UDP	A	501	-	20,26,26	0.79	1 (5%)	24,40,40	1.61	1 (4%)
3	GOL	A	502	-	5,5,5	0.20	0	5,5,5	0.38	0
2	UDP	B	501	-	20,26,26	0.80	0	24,40,40	1.70	3 (12%)
3	GOL	B	502	-	5,5,5	0.27	0	5,5,5	0.26	0
2	UDP	C	501	-	20,26,26	0.82	1 (5%)	24,40,40	1.71	4 (16%)
3	GOL	C	502	-	5,5,5	0.25	0	5,5,5	0.39	0
2	UDP	D	501	-	20,26,26	0.79	1 (5%)	24,40,40	1.39	2 (8%)
3	GOL	D	502	-	5,5,5	0.18	0	5,5,5	0.36	0
2	UDP	E	501	-	20,26,26	0.85	0	24,40,40	1.67	3 (12%)
3	GOL	E	502	-	5,5,5	0.20	0	5,5,5	0.38	0
2	UDP	F	501	-	20,26,26	0.86	1 (5%)	24,40,40	1.56	1 (4%)
3	GOL	F	502	-	5,5,5	0.23	0	5,5,5	0.46	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
2	UDP	A	501	-	-	0/12/32/32	0/2/2/2
3	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	UDP	B	501	-	-	0/12/32/32	0/2/2/2
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	UDP	C	501	-	-	0/12/32/32	0/2/2/2
3	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	UDP	D	501	-	-	0/12/32/32	0/2/2/2
3	GOL	D	502	-	-	0/4/4/4	0/0/0/0
2	UDP	E	501	-	-	0/12/32/32	0/2/2/2
3	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	UDP	F	501	-	-	0/12/32/32	0/2/2/2
3	GOL	F	502	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UDP	C2-N3	-2.17	1.33	1.38
2	D	501	UDP	C2-N3	-2.11	1.33	1.38
2	C	501	UDP	C2-N3	-2.02	1.34	1.38
2	F	501	UDP	O4'-C1'	2.07	1.44	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	UDP	C2'-C1'-N1	-2.18	107.62	113.46
2	D	501	UDP	O3B-PB-O2B	2.02	114.88	107.44
2	C	501	UDP	O3B-PB-O2B	2.17	115.41	107.44
2	B	501	UDP	O3B-PB-O2B	2.19	115.47	107.44
2	E	501	UDP	O3B-PB-O2B	2.23	115.61	107.44
2	E	501	UDP	O4'-C1'-N1	2.34	112.56	108.10
2	B	501	UDP	O4'-C1'-N1	2.46	112.78	108.10
2	C	501	UDP	O4'-C1'-N1	2.92	113.66	108.10
2	D	501	UDP	C4-N3-C2	5.44	119.94	114.21
2	F	501	UDP	C4-N3-C2	6.01	120.54	114.21
2	E	501	UDP	C4-N3-C2	6.34	120.89	114.21
2	C	501	UDP	C4-N3-C2	6.39	120.94	114.21
2	A	501	UDP	C4-N3-C2	6.57	121.13	114.21
2	B	501	UDP	C4-N3-C2	6.57	121.13	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	UDP	2	0
3	A	502	GOL	1	0
2	B	501	UDP	1	0
2	D	501	UDP	1	0
2	E	501	UDP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	365/402 (90%)	-0.16	0	100	100	18, 29, 41, 55	3 (0%)
1	B	365/402 (90%)	-0.16	0	100	100	19, 29, 43, 58	3 (0%)
1	C	365/402 (90%)	-0.08	1 (0%)	94	93	22, 36, 48, 57	3 (0%)
1	D	365/402 (90%)	0.03	2 (0%)	91	87	21, 38, 53, 63	3 (0%)
1	E	365/402 (90%)	-0.03	0	100	100	23, 37, 49, 58	3 (0%)
1	F	365/402 (90%)	0.06	2 (0%)	91	87	21, 38, 54, 72	3 (0%)
All	All	2190/2412 (90%)	-0.06	5 (0%)	95	94	18, 34, 50, 72	18 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	406	PRO	3.3
1	D	243	LEU	2.5
1	D	48	PHE	2.5
1	F	72	ASP	2.3
1	C	162	ALA	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	A	502	6/6	0.97	0.28	4.00	26,27,27,29	0
3	GOL	D	502	6/6	0.96	0.27	2.89	31,32,33,35	0
3	GOL	B	502	6/6	0.94	0.24	0.80	27,28,28,29	0
3	GOL	F	502	6/6	0.96	0.22	0.43	25,25,26,28	0
3	GOL	C	502	6/6	0.97	0.22	0.09	26,27,27,27	0
2	UDP	A	501	25/25	0.99	0.23	-0.03	28,32,34,34	0
3	GOL	E	502	6/6	0.97	0.23	-0.10	22,22,23,23	0
2	UDP	F	501	25/25	0.99	0.20	-0.50	25,31,33,34	0
2	UDP	E	501	25/25	0.98	0.21	-0.51	28,32,35,35	0
2	UDP	B	501	25/25	0.99	0.20	-0.65	32,37,41,41	0
2	UDP	C	501	25/25	0.97	0.20	-0.67	31,36,39,40	0
2	UDP	D	501	25/25	0.98	0.21	-0.96	30,38,43,47	0

6.5 Other polymers (i)

There are no such residues in this entry.