



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 AM GMT

PDB ID : 2F2H
Title : Structure of the YicI thiosugar Michaelis complex
Authors : Kim, Y.-W.; Lovering, A.L.; Strynadka, N.C.J.; Withers, S.G.
Deposited on : 2005-11-16
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

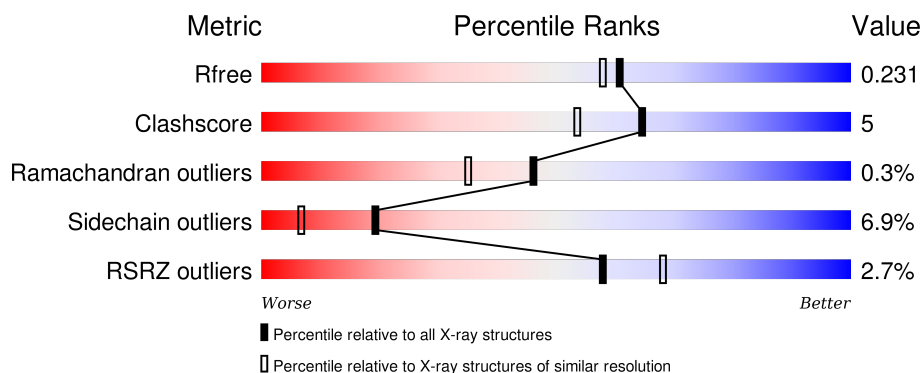
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 $\leq 5\%$. 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	773	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	B	773	<div> <div>3%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	C	773	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	D	773	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	E	773	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	773	

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
2	SO4	E	3009	-	-	-	X
2	SO4	F	3001	-	-	X	-
3	MPO	D	3012	-	-	-	X
3	MPO	E	3013	-	-	-	X
3	MPO	F	3014	-	-	-	X
4	XTG	F	3021	-	-	-	X
5	GOL	A	3024	-	-	-	X
5	GOL	A	3029	-	-	-	X
5	GOL	B	3026	-	-	-	X
5	GOL	D	3032	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39799 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	B	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	C	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	D	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	E	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	F	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			

There are 6 discrepancies between the modelled and reference sequences:

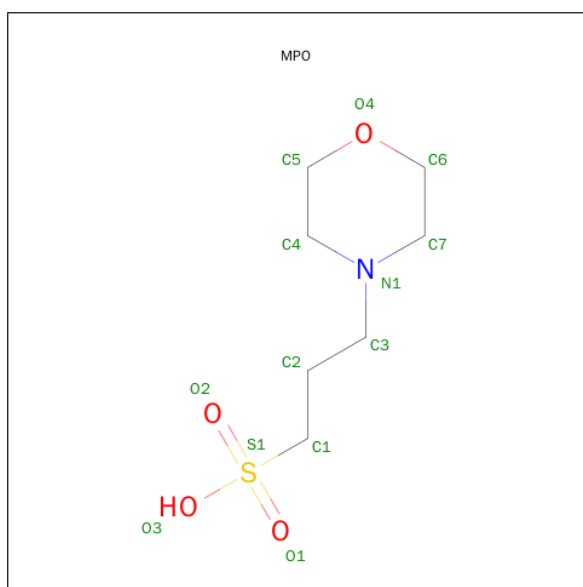
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	EXPRESSION TAG	UNP P31434
B	773	HIS	-	EXPRESSION TAG	UNP P31434
C	773	HIS	-	EXPRESSION TAG	UNP P31434
D	773	HIS	-	EXPRESSION TAG	UNP P31434
E	773	HIS	-	EXPRESSION TAG	UNP P31434
F	773	HIS	-	EXPRESSION TAG	UNP P31434

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



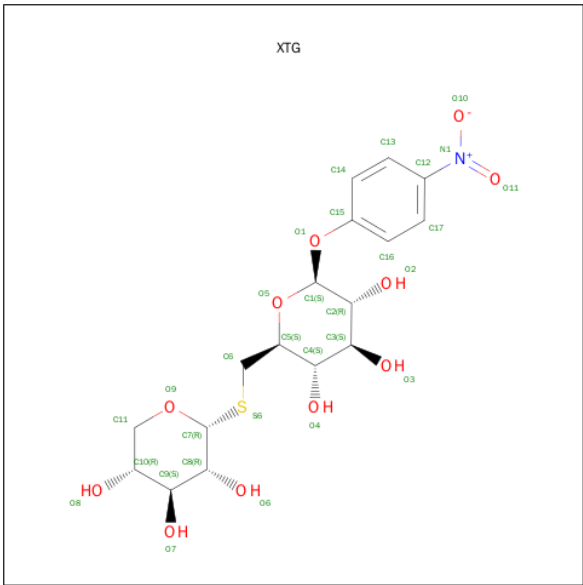
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



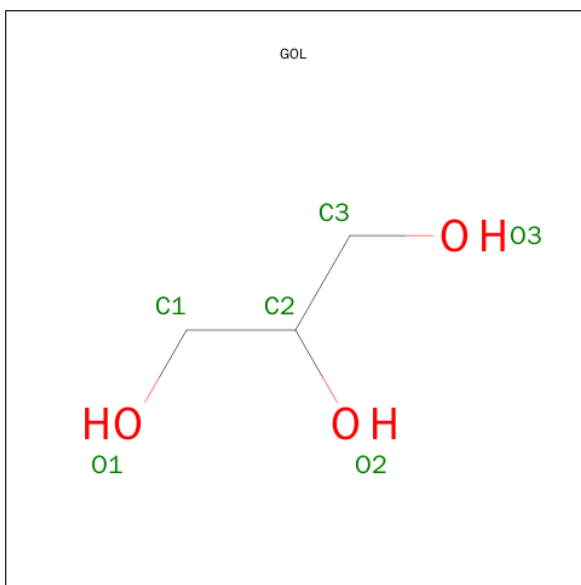
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	F	1	Total	C	N	O	S	5	0
			13	7	1	4	1		

- Molecule 4 is 4-NITROPHENYL 6-THIO-6-S-ALPHA-D-XYLOPYRANOSYL-BETA-D-G LUCOPYRANOSIDE (three-letter code: XTG) (formula: C₁₇H₂₃NO₁₁S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
4	B	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
4	C	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
4	D	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
4	E	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
4	F	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
4	F	1	Total	C	N	O	S	0	0
			30	17	1	11	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

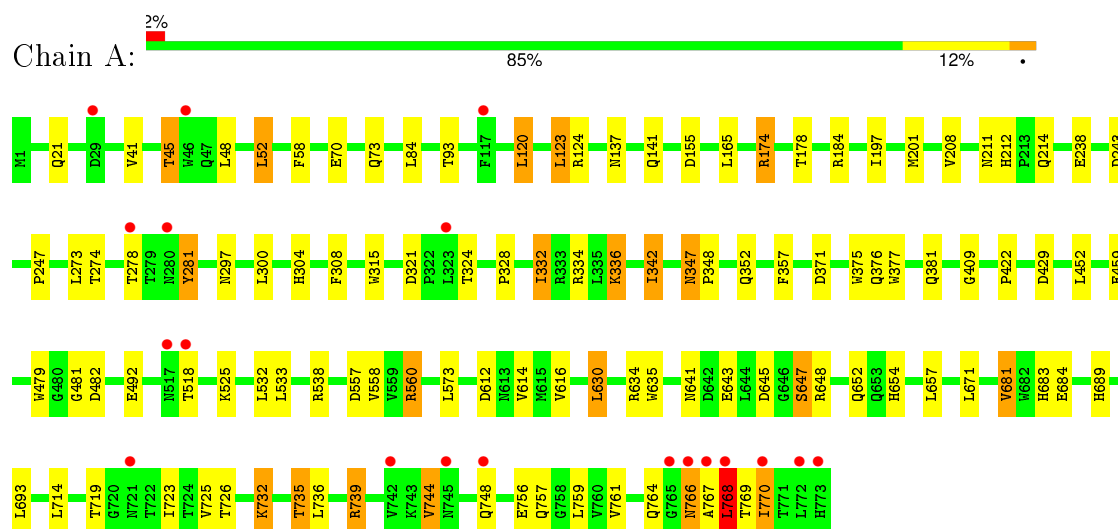
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	373	Total 373	O 373	0	0
6	B	290	Total 290	O 290	0	0
6	C	344	Total 344	O 344	0	0
6	D	370	Total 370	O 370	0	0
6	E	300	Total 300	O 300	0	0
6	F	326	Total 326	O 326	0	0

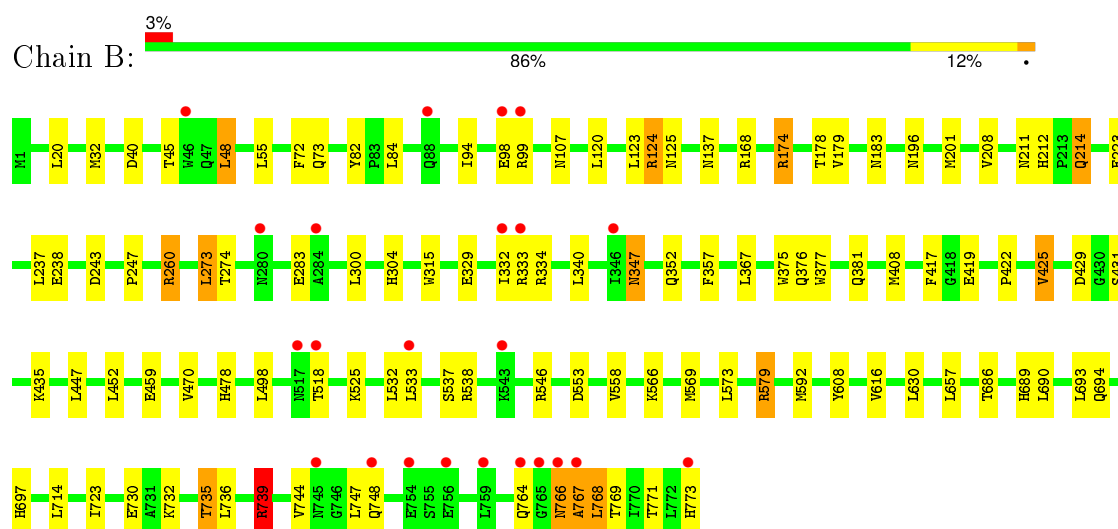
3 Residue-property plots [i](#)

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

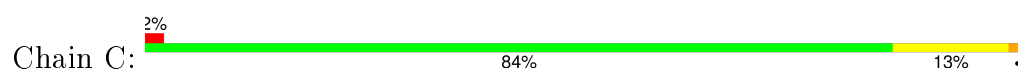
- Molecule 1: Putative family 31 glucosidase yicI

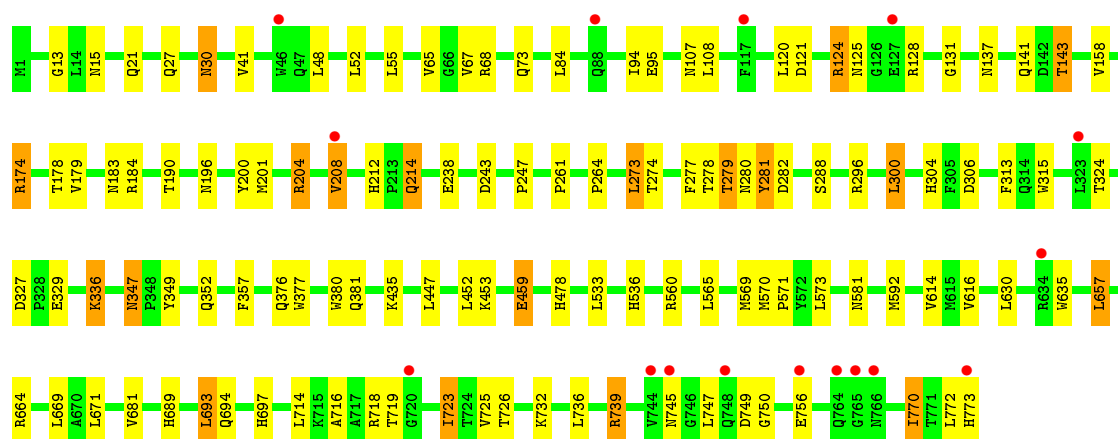


- Molecule 1: Putative family 31 glucosidase yicI

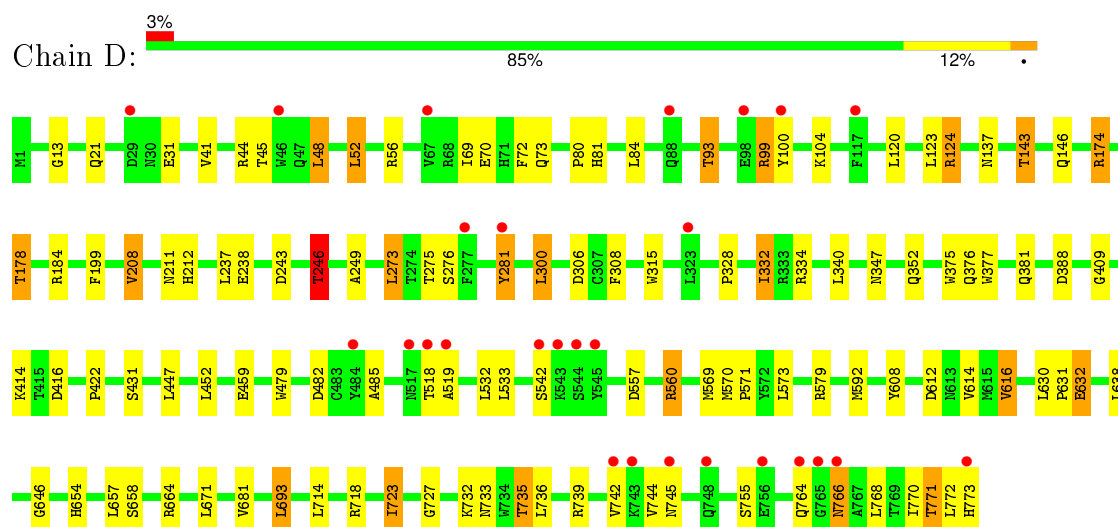


- Molecule 1: Putative family 31 glucosidase yicI

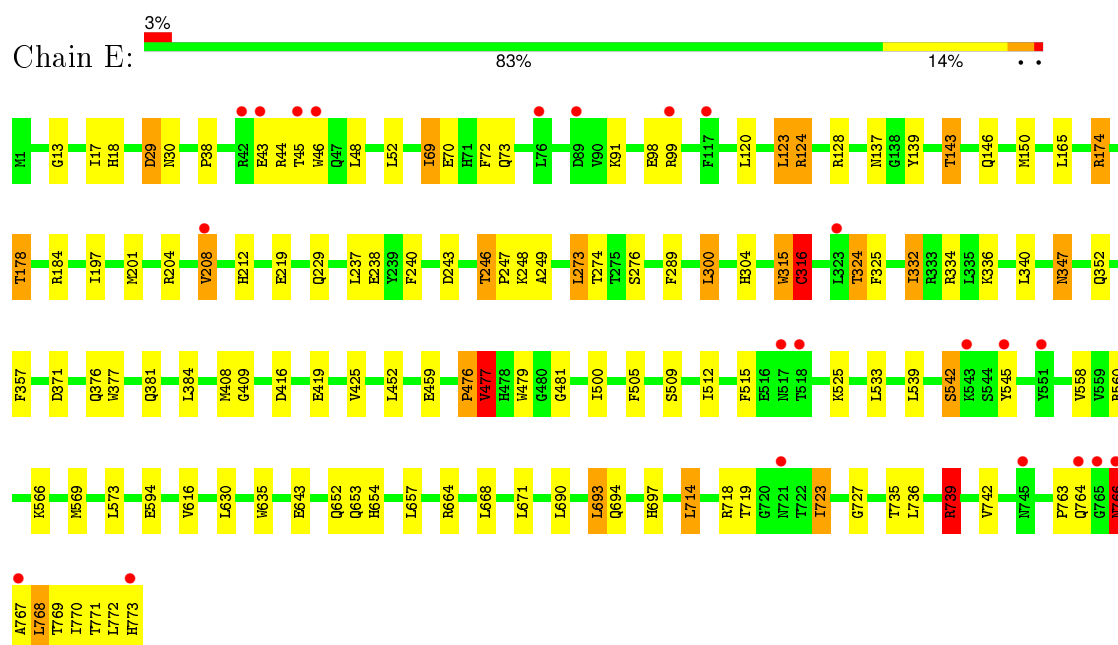




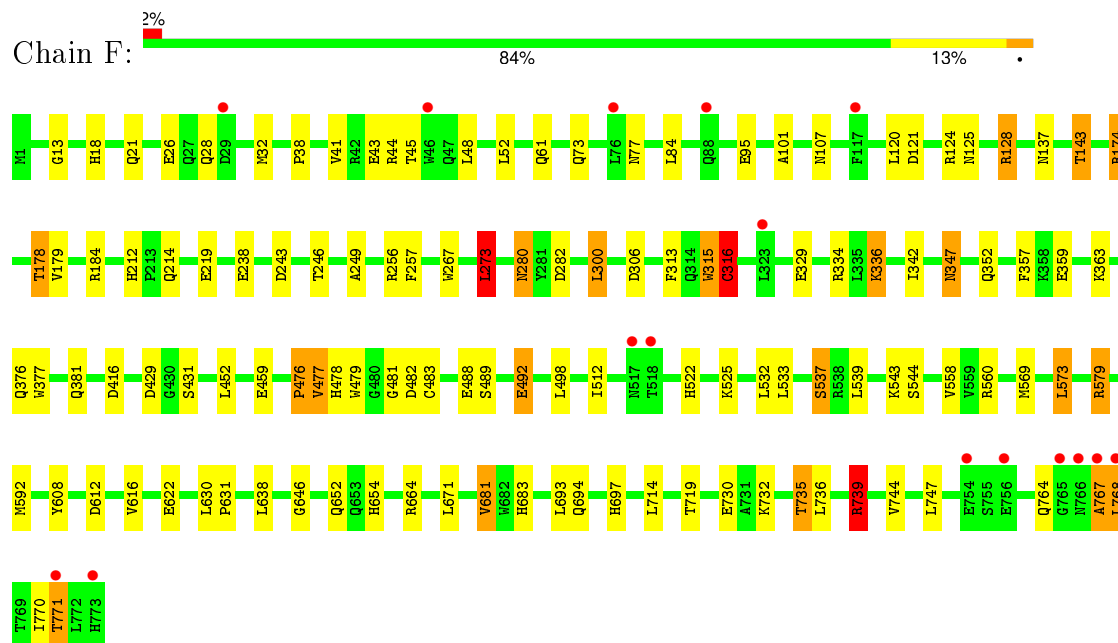
• Molecule 1: Putative family 31 glucosidase yicI



• Molecule 1: Putative family 31 glucosidase yicI



• Molecule 1: Putative family 31 glucosidase yicI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	162.32Å 175.84Å 210.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 1.95 28.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	86.4 (28.64-1.95) 86.4 (28.64-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.180 , 0.225 0.188 , 0.231	Depositor DCC
R_{free} test set	18828 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 375658 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	39799	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XTG, GOL, SO4, MPO

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	0.90	2/6416 (0.0%)	0.97	28/8719 (0.3%)
1	B	0.83	2/6416 (0.0%)	0.89	15/8719 (0.2%)
1	C	0.85	1/6416 (0.0%)	0.91	13/8719 (0.1%)
1	D	0.88	2/6416 (0.0%)	0.93	16/8719 (0.2%)
1	E	0.85	1/6416 (0.0%)	0.93	17/8719 (0.2%)
1	F	0.90	5/6416 (0.1%)	0.94	21/8719 (0.2%)
All	All	0.87	13/38496 (0.0%)	0.93	110/52314 (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	D	0	1
1	E	0	6
1	F	0	4
All	All	0	12

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	483	CYS	CB-SG	-8.95	1.67	1.82
1	F	537	SER	CB-OG	8.53	1.53	1.42
1	F	43	GLU	CG-CD	7.21	1.62	1.51
1	A	214	GLN	CB-CG	-6.47	1.35	1.52
1	C	336	LYS	CD-CE	6.32	1.67	1.51
1	D	632	GLU	CG-CD	6.29	1.61	1.51
1	F	329	GLU	CD-OE2	6.25	1.32	1.25
1	B	730	GLU	CD-OE2	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	GLU	CB-CG	-5.55	1.41	1.52
1	E	70	GLU	CB-CG	-5.52	1.41	1.52
1	D	664	ARG	CB-CG	-5.52	1.37	1.52
1	F	730	GLU	CG-CD	5.23	1.59	1.51
1	B	98	GLU	CG-CD	5.20	1.59	1.51

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	174	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	E	174	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	A	174	ARG	NE-CZ-NH2	-14.53	113.04	120.30
1	A	174	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	F	174	ARG	NE-CZ-NH2	-13.02	113.79	120.30
1	D	174	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	D	174	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	F	174	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	B	174	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	F	739	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	B	174	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	C	174	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	E	739	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	184	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	F	739	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	739	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	D	124	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	C	739	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	612	ASP	CB-CG-OD1	8.08	125.57	118.30
1	F	334	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	C	174	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	B	20	LEU	CA-CB-CG	7.88	133.42	115.30
1	D	664	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	F	334	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	739	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	560	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	E	739	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	F	128	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	F	560	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	F	316	CYS	N-CA-C	7.32	130.77	111.00
1	E	316	CYS	N-CA-C	7.29	130.68	111.00
1	B	579	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	334	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	D	612	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	184	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	E	739	ARG	CG-CD-NE	-6.99	97.13	111.80
1	E	124	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	F	579	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	E	560	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	E	184	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	739	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	F	579	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	F	128	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	D	739	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	560	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	E	477	VAL	N-CA-C	6.40	128.28	111.00
1	A	334	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	E	124	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	B	124	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	C	124	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	E	476	PRO	C-N-CA	6.18	137.14	121.70
1	A	52	LEU	CA-CB-CG	6.06	129.24	115.30
1	F	477	VAL	N-CA-C	6.05	127.33	111.00
1	A	334	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	124	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	538	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	647	SER	CB-CA-C	5.96	121.43	110.10
1	A	429	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	155	ASP	CB-CG-OD1	5.90	123.61	118.30
1	F	416	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	184	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	174	ARG	CD-NE-CZ	5.89	131.85	123.60
1	A	214	GLN	CB-CA-C	-5.88	98.65	110.40
1	A	560	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	739	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	184	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	664	ARG	N-CA-CB	-5.86	100.05	110.60
1	B	168	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	273	LEU	CA-CB-CG	5.83	128.70	115.30
1	F	184	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	371	ASP	CB-CG-OD1	5.80	123.53	118.30
1	E	476	PRO	CA-C-N	-5.78	104.49	117.20
1	F	739	ARG	CG-CD-NE	-5.77	99.68	111.80
1	A	630	LEU	CB-CG-CD1	5.77	120.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	123	LEU	CA-CB-CG	5.72	128.46	115.30
1	C	204	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	260	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	D	579	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	174	ARG	CD-NE-CZ	5.70	131.57	123.60
1	E	371	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	306	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	40	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	579	ARG	CG-CD-NE	-5.59	100.06	111.80
1	A	648	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	F	184	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	334	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	F	560	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	273	LEU	CA-CB-CG	5.50	127.95	115.30
1	D	560	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	739	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	184	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	52	LEU	CB-CG-CD2	5.34	120.08	111.00
1	C	327	ASP	CB-CG-OD1	5.32	123.08	118.30
1	F	273	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	120	LEU	CB-CG-CD2	5.29	119.99	111.00
1	A	174	ARG	CB-CG-CD	5.28	125.33	111.60
1	D	246	THR	N-CA-CB	-5.26	100.31	110.30
1	B	214	GLN	CB-CA-C	-5.24	99.92	110.40
1	C	282	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	123	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	579	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	630	LEU	CA-CB-CG	5.12	127.09	115.30
1	F	664	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	52	LEU	CA-CB-CG	5.10	127.03	115.30
1	C	657	LEU	CB-CG-CD1	5.05	119.58	111.00
1	F	612	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	538	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	342	ILE	CG1-CB-CG2	-5.01	100.38	111.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	ASN	Peptide
1	D	766	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	315	TRP	Mainchain,Peptide
1	E	476	PRO	Mainchain,Peptide
1	E	763	PRO	Peptide
1	E	766	ASN	Peptide
1	F	315	TRP	Mainchain,Peptide
1	F	476	PRO	Mainchain,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	6232	0	5939	63	0
1	B	6232	0	5939	59	0
1	C	6232	0	5939	65	0
1	D	6232	0	5939	74	0
1	E	6232	0	5939	71	0
1	F	6232	0	5939	67	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	10	0	0	1	0
2	F	15	0	0	3	0
3	B	13	0	15	0	0
3	C	13	0	15	0	0
3	D	13	0	15	0	0
3	E	13	0	15	0	0
3	F	13	0	15	0	0
4	A	30	0	23	2	0
4	B	30	0	23	1	0
4	C	30	0	23	0	0
4	D	30	0	23	7	0
4	E	30	0	23	1	0
4	F	60	0	46	1	0
5	A	18	0	24	5	0
5	B	12	0	16	2	0
5	C	18	0	24	1	0
5	D	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	12	0	16	0	0
5	F	12	0	16	1	0
6	A	373	0	0	4	0
6	B	290	0	0	4	0
6	C	344	0	0	6	0
6	D	370	0	0	10	0
6	E	300	0	0	9	0
6	F	326	0	0	6	0
All	All	39799	0	35982	379	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 5.

All (379) 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:A:124:ARG:NH2	1:A:243:ASP:OD1	1.88	1.04
1:D:569:MET:HE2	1:D:638:LEU:HD21	1.51	0.91
1:B:32:MET:CE	1:B:94:ILE:HG23	2.03	0.89
1:C:30:ASN:HD22	1:C:30:ASN:H	1.19	0.88
1:C:352:GLN:NE2	1:D:73:GLN:H	1.72	0.86
1:D:352:GLN:HE21	1:D:376:GLN:HE22	1.24	0.85
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.57	0.85
1:C:352:GLN:HE22	1:D:73:GLN:H	1.23	0.84
1:C:352:GLN:HE21	1:C:376:GLN:HE22	1.28	0.81
1:C:158:VAL:O	1:C:204:ARG:NH2	2.13	0.81
1:C:13:GLY:O	1:C:143:THR:HB	1.81	0.80
1:D:70:GLU:OE1	6:D:3123:HOH:O	1.99	0.79
1:F:212:HIS:HE1	1:F:238:GLU:H	1.28	0.79
1:E:204:ARG:NH2	6:E:3297:HOH:O	2.15	0.78
1:F:246:THR:HG21	2:F:3001:SO4:O3	1.86	0.75
4:B:3016:XTG:H14	1:F:48:LEU:HD11	1.66	0.75
1:D:727:GLY:H	1:D:766:ASN:HD21	1.35	0.74
1:A:352:GLN:NE2	1:B:73:GLN:H	1.85	0.74
1:A:352:GLN:HE22	1:B:73:GLN:H	1.35	0.74
1:D:569:MET:CE	1:D:638:LEU:CD2	2.66	0.73
1:A:201:MET:HE1	1:A:247:PRO:HB3	1.71	0.73
1:D:569:MET:CE	1:D:638:LEU:HD21	2.18	0.72
1:B:352:GLN:HE21	1:B:376:GLN:HE22	1.37	0.72
1:A:352:GLN:HE21	1:A:376:GLN:HE22	1.36	0.72
1:B:566:LYS:HA	1:B:569:MET:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ASN:HD21	1:A:739:ARG:HH21	1.36	0.71
1:A:141:GLN:CD	6:A:3289:HOH:O	2.27	0.71
1:B:332:ILE:CD1	1:B:408:MET:O	2.39	0.71
1:B:211:ASN:ND2	5:B:3026:GOL:H32	2.07	0.69
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.73	0.69
1:F:306:ASP:OD1	6:F:3038:HOH:O	2.10	0.69
1:A:212:HIS:HE1	1:A:238:GLU:H	1.40	0.68
1:F:13:GLY:O	1:F:143:THR:HB	1.93	0.68
1:F:719:THR:HG22	6:F:3241:HOH:O	1.93	0.68
1:D:352:GLN:NE2	1:E:73:GLN:H	1.92	0.67
1:B:332:ILE:HD12	1:B:333:ARG:N	2.10	0.66
1:D:306:ASP:OD2	4:D:3018:XTG:H112	1.96	0.66
1:B:211:ASN:HD21	5:B:3026:GOL:H32	1.61	0.66
1:C:30:ASN:ND2	1:C:30:ASN:H	1.93	0.65
1:E:347:ASN:C	1:E:347:ASN:HD22	2.00	0.65
1:E:723:ILE:HG12	1:E:770:ILE:HB	1.79	0.65
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.32	0.65
1:A:73:GLN:H	1:F:352:GLN:HE22	1.45	0.65
1:B:212:HIS:HE1	1:B:238:GLU:H	1.44	0.65
1:D:681:VAL:HG13	1:D:681:VAL:O	1.96	0.65
1:B:32:MET:HE3	1:B:94:ILE:HG23	1.77	0.65
1:E:300:LEU:HD13	1:E:340:LEU:HD21	1.77	0.64
1:A:45:THR:HB	1:F:543:LYS:HZ1	1.62	0.64
1:D:93:THR:HG22	1:D:104:LYS:HB3	1.78	0.64
1:C:296:ARG:O	1:C:560:ARG:NH1	2.30	0.64
1:F:280:ASN:HD22	1:F:282:ASP:H	1.43	0.63
1:E:336:LYS:HE2	1:E:409:GLY:O	1.98	0.63
1:A:73:GLN:H	1:F:352:GLN:NE2	1.95	0.63
1:F:212:HIS:CE1	1:F:238:GLU:H	2.14	0.63
1:A:211:ASN:ND2	5:A:3029:GOL:H32	2.12	0.63
1:A:525:LYS:HG2	1:A:558:VAL:HG21	1.81	0.63
1:D:744:VAL:HG21	1:D:770:ILE:HG23	1.81	0.63
1:E:212:HIS:HE1	1:E:238:GLU:H	1.47	0.62
1:E:566:LYS:HA	1:E:569:MET:HE2	1.81	0.62
1:D:246:THR:HG22	1:D:249:ALA:CB	2.29	0.62
1:E:143:THR:HG22	6:E:3181:HOH:O	1.99	0.62
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.82	0.62
1:C:770:ILE:HD11	1:C:772:LEU:HD13	1.81	0.62
1:F:178:THR:CG2	6:F:3256:HOH:O	2.48	0.62
1:D:212:HIS:HE1	1:D:238:GLU:H	1.48	0.61
1:E:315:TRP:H	1:E:381:GLN:HE21	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:GLY:O	1:E:143:THR:HB	2.01	0.61
1:A:281:TYR:O	1:A:324:THR:HG23	2.00	0.61
1:C:212:HIS:HE1	1:C:238:GLU:H	1.46	0.61
1:F:767:ALA:O	1:F:768:LEU:C	2.38	0.60
1:A:641:ASN:ND2	1:A:739:ARG:HH21	1.98	0.60
1:E:246:THR:HG23	1:E:249:ALA:H	1.67	0.60
1:F:336:LYS:HD2	1:F:342:ILE:HD12	1.83	0.60
1:B:283:GLU:OE1	1:B:334:ARG:HD2	2.01	0.60
1:A:744:VAL:HG21	1:A:770:ILE:HD13	1.83	0.60
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.83	0.60
1:D:352:GLN:NE2	1:D:376:GLN:HE22	1.96	0.59
1:E:352:GLN:HE21	1:E:376:GLN:HE22	1.49	0.59
1:E:332:ILE:HD11	1:E:409:GLY:HA3	1.83	0.59
1:F:280:ASN:ND2	1:F:282:ASP:H	1.99	0.59
1:C:716:ALA:HB1	1:C:723:ILE:HD13	1.85	0.59
1:A:93:THR:HA	5:A:3024:GOL:H12	1.84	0.58
1:F:735:THR:CG2	6:F:3193:HOH:O	2.50	0.58
1:A:681:VAL:HG23	1:A:683:HIS:CE1	2.39	0.58
1:B:124:ARG:HD3	1:B:243:ASP:OD1	2.04	0.58
1:F:347:ASN:C	1:F:347:ASN:HD22	2.07	0.58
1:C:214:GLN:HG3	1:C:435:LYS:HG2	1.86	0.58
1:B:352:GLN:NE2	1:B:376:GLN:HE22	2.01	0.57
1:D:211:ASN:ND2	5:D:3032:GOL:H32	2.20	0.57
1:F:489:SER:HA	1:F:492:GLU:HG3	1.86	0.57
1:C:124:ARG:HD3	1:C:243:ASP:OD1	2.03	0.57
1:C:73:GLN:H	1:E:352:GLN:NE2	2.01	0.57
1:B:735:THR:HG23	6:B:3294:HOH:O	2.04	0.57
1:C:121:ASP:OD1	1:C:128:ARG:NH2	2.37	0.57
1:F:61:GLN:NE2	1:F:257:PHE:HA	2.20	0.57
1:D:13:GLY:O	1:D:143:THR:HB	2.04	0.57
1:C:274:THR:HG22	1:C:304:HIS:HB3	1.87	0.57
1:E:124:ARG:HD3	1:E:243:ASP:OD1	2.05	0.57
1:E:727:GLY:H	1:E:766:ASN:HD21	1.50	0.57
1:B:690:LEU:O	1:B:739:ARG:HB2	2.05	0.56
1:D:735:THR:CG2	6:D:3161:HOH:O	2.54	0.56
1:B:352:GLN:NE2	1:F:73:GLN:H	2.04	0.56
1:D:485:ALA:CB	1:D:519:ALA:HB2	2.34	0.56
1:A:725:VAL:HB	1:A:768:LEU:HB3	1.88	0.56
1:E:315:TRP:H	1:E:381:GLN:NE2	2.04	0.55
1:A:352:GLN:NE2	1:A:376:GLN:HE22	2.03	0.55
1:F:61:GLN:HE22	1:F:256:ARG:C	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ASN:C	1:C:347:ASN:HD22	2.10	0.55
1:C:723:ILE:HD11	1:C:725:VAL:HG22	1.88	0.55
1:E:18:HIS:O	1:E:38:PRO:HA	2.07	0.55
1:E:246:THR:HG21	2:E:3004:SO4:O4	2.06	0.55
1:E:352:GLN:NE2	1:E:376:GLN:HE22	2.05	0.55
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.87	0.55
1:A:744:VAL:CG2	1:A:770:ILE:HD13	2.37	0.55
1:F:478:HIS:HD2	6:F:3069:HOH:O	1.89	0.55
1:C:128:ARG:HH22	1:C:131:GLY:HA3	1.72	0.54
1:A:347:ASN:C	1:A:347:ASN:HD22	2.10	0.54
1:D:352:GLN:HE22	1:E:73:GLN:H	1.55	0.54
1:F:488:GLU:O	1:F:492:GLU:HG2	2.08	0.54
1:A:328:PRO:O	1:A:332:ILE:HG23	2.08	0.54
1:D:124:ARG:HD3	1:D:243:ASP:OD1	2.07	0.54
1:C:352:GLN:NE2	1:C:376:GLN:HE22	2.02	0.54
1:B:429:ASP:OD1	1:B:431:SER:OG	2.23	0.54
1:D:178:THR:CG2	6:D:3276:HOH:O	2.54	0.54
1:D:21:GLN:HE22	1:D:41:VAL:H	1.55	0.54
1:A:641:ASN:HD21	1:A:739:ARG:NH2	2.05	0.54
1:D:212:HIS:CE1	1:D:238:GLU:H	2.26	0.53
1:F:352:GLN:HE21	1:F:376:GLN:HE22	1.54	0.53
1:C:347:ASN:ND2	1:C:349:TYR:H	2.06	0.53
1:F:681:VAL:HG23	1:F:683:HIS:CE1	2.44	0.53
1:D:275:THR:O	1:D:276:SER:HB2	2.08	0.53
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.91	0.53
1:C:107:ASN:ND2	1:C:125:ASN:HD21	2.07	0.53
1:C:73:GLN:H	1:E:352:GLN:HE22	1.57	0.52
1:C:719:THR:HG22	6:C:3086:HOH:O	2.08	0.52
1:E:512:ILE:HB	1:E:539:LEU:HD23	1.91	0.52
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.90	0.52
1:D:246:THR:HG22	1:D:249:ALA:HB2	1.90	0.52
1:B:212:HIS:CE1	1:B:238:GLU:H	2.27	0.52
1:D:300:LEU:HD13	1:D:340:LEU:HD21	1.90	0.52
1:E:347:ASN:ND2	1:E:347:ASN:C	2.62	0.52
5:A:3029:GOL:H31	6:A:3127:HOH:O	2.09	0.52
1:B:767:ALA:O	1:B:768:LEU:O	2.28	0.52
1:C:329:GLU:HB2	6:C:3243:HOH:O	2.09	0.52
1:C:459:GLU:H	1:C:459:GLU:CD	2.13	0.52
1:F:124:ARG:HD3	1:F:243:ASP:OD1	2.10	0.52
1:E:212:HIS:CE1	1:E:238:GLU:H	2.26	0.52
1:D:482:ASP:OD2	4:D:3018:XTG:H62	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:LEU:O	1:F:48:LEU:HD12	2.10	0.51
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.45	0.51
1:F:429:ASP:OD1	1:F:431:SER:OG	2.25	0.51
1:B:352:GLN:HE22	1:F:73:GLN:H	1.57	0.51
1:B:367:LEU:HD11	1:B:425:VAL:HG13	1.92	0.51
1:D:447:LEU:C	1:D:447:LEU:HD23	2.30	0.51
1:A:315:TRP:H	1:A:381:GLN:HE21	1.57	0.51
1:F:246:THR:HG23	1:F:249:ALA:H	1.76	0.51
1:E:212:HIS:HD2	6:E:3148:HOH:O	1.94	0.51
1:B:447:LEU:C	1:B:447:LEU:HD23	2.31	0.51
1:D:93:THR:CG2	6:D:3217:HOH:O	2.58	0.51
1:E:45:THR:HG23	1:E:46:TRP:CD1	2.46	0.51
1:D:352:GLN:HE22	1:E:72:PHE:HA	1.76	0.50
1:B:329:GLU:HA	1:B:332:ILE:HG13	1.92	0.50
1:B:375:TRP:CE2	1:B:422:PRO:HG3	2.46	0.50
1:B:332:ILE:HD13	1:B:408:MET:O	2.11	0.50
1:B:735:THR:CG2	6:B:3294:HOH:O	2.60	0.50
1:B:55:LEU:N	1:B:55:LEU:HD12	2.27	0.50
1:F:482:ASP:OD2	4:F:3020:XTG:H62	2.11	0.50
1:C:478:HIS:HE1	6:C:3149:HOH:O	1.95	0.50
1:D:723:ILE:HG12	1:D:770:ILE:HB	1.93	0.50
1:E:123:LEU:HD12	1:E:128:ARG:HA	1.92	0.50
1:E:324:THR:HG23	1:E:325:PHE:CD2	2.47	0.50
1:B:478:HIS:HD2	6:B:3236:HOH:O	1.93	0.50
1:C:723:ILE:HD11	1:C:725:VAL:CG2	2.42	0.49
1:F:61:GLN:HE22	1:F:257:PHE:N	2.09	0.49
1:A:278:THR:HG21	1:B:45:THR:HA	1.94	0.49
1:C:279:THR:O	1:D:44:ARG:NH2	2.44	0.49
1:B:201:MET:CE	1:B:247:PRO:HB3	2.42	0.49
1:E:416:ASP:OD2	4:E:3019:XTG:H8	2.13	0.49
1:C:447:LEU:HD23	1:C:447:LEU:C	2.33	0.49
1:F:638:LEU:O	1:F:739:ARG:NH2	2.44	0.49
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.47	0.49
1:A:641:ASN:HD21	1:A:739:ARG:HE	1.60	0.49
1:B:32:MET:HE2	1:B:94:ILE:CG2	2.36	0.49
1:D:306:ASP:OD1	4:D:3018:XTG:O8	2.13	0.49
1:D:332:ILE:HD11	1:D:409:GLY:HA3	1.95	0.49
1:C:212:HIS:CE1	1:C:238:GLU:H	2.29	0.48
1:E:43:GLU:H	1:E:43:GLU:CD	2.16	0.48
1:E:300:LEU:HD13	1:E:340:LEU:CD2	2.43	0.48
1:A:238:GLU:OE1	5:A:3029:GOL:H32	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:CE1	1:A:238:GLU:H	2.26	0.48
1:F:178:THR:HB	1:F:219:GLU:OE1	2.14	0.48
1:C:15:ASN:HD22	1:C:141:GLN:NE2	2.12	0.48
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.13	0.48
1:D:306:ASP:OD2	4:D:3018:XTG:C11	2.61	0.48
1:A:332:ILE:HD11	1:A:409:GLY:HA3	1.95	0.48
1:A:281:TYR:CZ	1:A:308:PHE:HB2	2.49	0.48
1:C:478:HIS:HD2	6:C:3063:HOH:O	1.96	0.48
1:F:246:THR:HG21	2:F:3001:SO4:S	2.54	0.48
1:D:81:HIS:HB2	6:D:3206:HOH:O	2.14	0.48
1:A:315:TRP:H	1:A:381:GLN:NE2	2.11	0.48
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.96	0.48
1:F:681:VAL:HG12	2:F:3003:SO4:O3	2.14	0.47
1:B:332:ILE:HG12	1:B:408:MET:O	2.14	0.47
1:E:693:LEU:HD13	1:E:718:ARG:HB2	1.95	0.47
1:B:201:MET:HE1	1:B:247:PRO:HB3	1.96	0.47
1:A:482:ASP:OD2	4:A:3015:XTG:H62	2.12	0.47
1:A:58:PHE:CZ	5:A:3028:GOL:H12	2.49	0.47
1:C:30:ASN:HD22	1:C:30:ASN:N	1.93	0.47
1:E:332:ILE:CD1	1:E:409:GLY:HA3	2.44	0.47
1:E:332:ILE:HD12	1:E:332:ILE:C	2.35	0.47
1:A:770:ILE:C	1:A:770:ILE:HD12	2.34	0.47
1:D:557:ASP:OD1	1:D:560:ARG:NH2	2.47	0.47
1:E:212:HIS:CE1	1:E:237:LEU:HD12	2.50	0.47
1:B:329:GLU:O	1:B:332:ILE:HG13	2.15	0.47
1:F:347:ASN:C	1:F:347:ASN:ND2	2.68	0.47
1:F:315:TRP:H	1:F:381:GLN:NE2	2.12	0.47
1:B:766:ASN:ND2	6:B:3171:HOH:O	2.47	0.47
1:D:485:ALA:HB1	1:D:519:ALA:CB	2.44	0.47
1:F:32:MET:HE2	1:F:101:ALA:HB1	1.97	0.47
1:F:352:GLN:NE2	1:F:376:GLN:HE22	2.13	0.46
1:D:735:THR:HG22	6:D:3161:HOH:O	2.16	0.46
1:D:199:PHE:HA	1:D:208:VAL:O	2.15	0.46
1:E:17:ILE:CG1	1:E:139:TYR:HB3	2.45	0.46
1:C:352:GLN:HE22	1:D:73:GLN:N	2.01	0.46
1:C:27:GLN:HG3	1:C:94:ILE:HD13	1.97	0.46
1:A:274:THR:HG22	1:A:304:HIS:HB3	1.97	0.46
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.97	0.46
1:E:735:THR:HG22	6:E:3178:HOH:O	2.15	0.46
1:A:761:VAL:CG1	1:A:768:LEU:HD21	2.46	0.46
1:E:143:THR:CG2	6:E:3181:HOH:O	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:GLU:CD	1:F:28:GLN:HE21	2.19	0.46
1:A:45:THR:HB	1:F:543:LYS:NZ	2.29	0.46
1:B:766:ASN:O	1:B:767:ALA:HB2	2.16	0.46
1:E:248:LYS:NZ	1:E:594:GLU:OE1	2.49	0.46
1:A:70:GLU:HG3	6:A:3251:HOH:O	2.15	0.46
1:E:477:VAL:HG11	1:E:509:SER:HB2	1.97	0.46
1:A:21:GLN:NE2	1:A:41:VAL:H	2.13	0.46
4:A:3015:XTG:C14	1:B:48:LEU:HD11	2.46	0.46
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.98	0.46
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.40	0.46
1:E:274:THR:HG22	1:E:304:HIS:HB3	1.98	0.45
1:F:267:TRP:HD1	5:F:3022:GOL:HO3	1.63	0.45
1:D:479:TRP:HH2	4:D:3018:XTG:HO7	1.64	0.45
1:A:767:ALA:O	1:A:769:THR:N	2.49	0.45
1:B:498:LEU:HD21	1:B:608:TYR:HB3	1.97	0.45
1:A:336:LYS:HE2	1:A:409:GLY:O	2.17	0.45
1:B:767:ALA:O	1:B:768:LEU:C	2.54	0.45
1:F:512:ILE:HB	1:F:539:LEU:HD23	1.99	0.45
1:E:204:ARG:HG3	6:E:3297:HOH:O	2.15	0.45
1:F:107:ASN:HD22	1:F:125:ASN:HD21	1.64	0.45
1:E:91:LYS:CE	6:E:3177:HOH:O	2.64	0.45
1:C:380:TRP:CZ3	1:D:48:LEU:HD13	2.51	0.45
1:D:93:THR:HG23	6:D:3217:HOH:O	2.15	0.45
1:F:479:TRP:CZ3	1:F:481:GLY:HA2	2.52	0.45
1:A:297:ASN:O	1:A:560:ARG:HD3	2.17	0.45
1:C:65:VAL:HG12	1:C:108:LEU:CD2	2.46	0.45
1:C:67:VAL:O	1:C:238:GLU:HA	2.17	0.45
1:A:21:GLN:HE22	1:A:41:VAL:H	1.64	0.45
1:A:767:ALA:C	1:A:769:THR:N	2.71	0.45
1:B:214:GLN:HG3	1:B:435:LYS:HG2	1.98	0.45
1:D:238:GLU:OE1	5:D:3032:GOL:H32	2.17	0.45
1:B:315:TRP:H	1:B:381:GLN:HE21	1.62	0.45
1:F:315:TRP:H	1:F:381:GLN:HE21	1.64	0.44
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.64	0.44
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.98	0.44
1:B:300:LEU:HD12	1:B:340:LEU:HD21	1.99	0.44
1:C:281:TYR:O	1:C:324:THR:CG2	2.66	0.44
1:E:289:PHE:HZ	1:E:545:TYR:CD1	2.34	0.44
1:D:654:HIS:ND1	1:D:658:SER:OG	2.36	0.44
1:A:352:GLN:HE22	1:B:72:PHE:HA	1.82	0.44
1:F:336:LYS:HD2	1:F:342:ILE:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:VAL:CG1	1:E:509:SER:HB2	2.48	0.44
1:B:107:ASN:ND2	1:B:125:ASN:HD21	2.15	0.44
1:E:635:TRP:O	1:E:643:GLU:HA	2.18	0.44
1:E:515:PHE:O	1:E:542:SER:HB2	2.17	0.44
1:C:30:ASN:N	1:C:30:ASN:ND2	2.61	0.44
1:B:274:THR:HG22	1:B:304:HIS:HB3	1.99	0.44
1:E:668:LEU:HD21	1:E:714:LEU:HD13	1.99	0.44
1:D:328:PRO:O	1:D:332:ILE:HG23	2.18	0.44
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.32	0.44
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.53	0.44
1:E:479:TRP:CZ3	1:E:481:GLY:HA2	2.53	0.44
1:C:570:MET:N	1:C:571:PRO:CD	2.81	0.44
1:A:748:GLN:HG2	1:A:769:THR:CG2	2.47	0.43
1:C:565:LEU:O	1:C:569:MET:HG3	2.18	0.43
1:E:178:THR:CG2	6:E:3308:HOH:O	2.66	0.43
1:C:689:HIS:ND1	1:C:739:ARG:HD3	2.33	0.43
1:B:212:HIS:CE1	1:B:237:LEU:HD12	2.53	0.43
1:F:313:PHE:HA	1:F:381:GLN:NE2	2.33	0.43
1:C:261:PRO:O	1:C:581:ASN:HA	2.18	0.43
1:E:165:LEU:HA	1:E:197:ILE:O	2.18	0.43
1:D:414:LYS:HZ3	4:D:3018:XTG:H10	1.84	0.43
1:D:744:VAL:HG22	1:D:771:THR:O	2.18	0.43
1:E:767:ALA:O	1:E:768:LEU:C	2.57	0.43
1:D:123:LEU:HD22	1:D:123:LEU:N	2.34	0.43
1:D:570:MET:N	1:D:571:PRO:CD	2.82	0.43
1:D:300:LEU:HD13	1:D:340:LEU:CD2	2.49	0.43
1:C:315:TRP:H	1:C:381:GLN:NE2	2.17	0.43
1:D:246:THR:HG21	2:D:3002:SO4:O2	2.19	0.43
1:A:635:TRP:O	1:A:643:GLU:HA	2.18	0.43
1:C:693:LEU:HD13	1:C:718:ARG:HB2	2.01	0.43
1:C:352:GLN:HE22	1:D:72:PHE:HA	1.84	0.42
1:C:635:TRP:CH2	1:C:664:ARG:HG2	2.54	0.42
1:D:31:GLU:OE1	1:D:56:ARG:HD3	2.19	0.42
1:F:61:GLN:NE2	1:F:257:PHE:CA	2.82	0.42
1:A:557:ASP:OD1	1:A:560:ARG:NH2	2.52	0.42
1:E:69:ILE:HG12	1:E:150:MET:CE	2.49	0.42
1:D:375:TRP:CE2	1:D:422:PRO:HG3	2.54	0.42
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.55	0.42
1:A:321:ASP:OD1	1:A:321:ASP:C	2.58	0.42
1:D:681:VAL:CG1	1:D:681:VAL:O	2.66	0.42
1:A:281:TYR:O	1:A:324:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HA	1:A:197:ILE:O	2.20	0.42
1:D:212:HIS:CE1	1:D:237:LEU:HD12	2.55	0.42
5:C:3023:GOL:H12	6:C:3365:HOH:O	2.19	0.42
1:F:735:THR:HG23	6:F:3193:HOH:O	2.17	0.42
1:F:631:PRO:O	1:F:646:GLY:HA3	2.19	0.42
1:A:634:ARG:NH2	1:A:645:ASP:OD1	2.53	0.42
1:F:498:LEU:HD21	1:F:608:TYR:HB3	2.00	0.42
1:C:536:HIS:HA	6:C:3099:HOH:O	2.19	0.42
1:F:18:HIS:O	1:F:38:PRO:HA	2.19	0.42
1:C:200:TYR:CZ	1:C:208:VAL:HG13	2.54	0.42
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.68	0.42
1:D:178:THR:HG23	6:D:3276:HOH:O	2.19	0.42
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.55	0.41
1:D:416:ASP:OD2	4:D:3018:XTG:H8	2.20	0.41
1:D:143:THR:CG2	6:D:3311:HOH:O	2.68	0.41
1:E:219:GLU:HB2	1:E:229:GLN:HB3	2.02	0.41
1:F:121:ASP:OD1	1:F:128:ARG:HD2	2.20	0.41
1:E:273:LEU:HB2	1:E:300:LEU:HD21	2.02	0.41
1:B:748:GLN:O	1:B:768:LEU:HA	2.20	0.41
1:C:313:PHE:CA	1:C:381:GLN:HE22	2.33	0.41
1:E:690:LEU:O	1:E:739:ARG:HB2	2.19	0.41
1:E:201:MET:HE1	1:E:247:PRO:HB3	2.02	0.41
1:D:99:ARG:NH2	1:D:100:TYR:OH	2.53	0.41
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.55	0.41
1:F:525:LYS:HG2	1:F:558:VAL:HG21	2.03	0.41
1:E:48:LEU:N	1:E:48:LEU:HD23	2.36	0.41
1:C:183:ASN:HA	1:C:196:ASN:ND2	2.36	0.41
1:E:29:ASP:HB3	1:E:30:ASN:H	1.73	0.41
1:F:768:LEU:HA	1:F:768:LEU:HD12	1.82	0.41
1:B:347:ASN:HD22	1:B:347:ASN:C	2.24	0.41
1:D:281:TYR:CZ	1:D:308:PHE:HB2	2.56	0.41
1:F:522:HIS:CB	1:F:622:GLU:HG3	2.50	0.41
1:B:82:TYR:CD1	1:B:470:VAL:HB	2.55	0.41
1:F:569:MET:HB2	1:F:573:LEU:HD22	2.03	0.41
1:C:747:LEU:HD22	1:C:750:GLY:O	2.20	0.41
1:B:748:GLN:HB2	1:B:769:THR:HB	2.03	0.41
1:A:748:GLN:HB2	1:A:769:THR:HG22	2.03	0.41
1:B:223:GLU:O	1:C:190:THR:HA	2.20	0.41
1:A:375:TRP:CE2	1:A:422:PRO:HG3	2.56	0.41
1:F:21:GLN:NE2	1:F:41:VAL:H	2.19	0.41
1:C:128:ARG:NH2	1:C:131:GLY:HA3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ASN:ND2	1:C:347:ASN:C	2.73	0.41
1:D:631:PRO:O	1:D:646:GLY:HA3	2.21	0.41
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.56	0.41
1:D:388:ASP:OD1	1:D:388:ASP:C	2.59	0.41
1:A:342:ILE:HD12	1:A:342:ILE:N	2.36	0.41
1:C:55:LEU:HA	1:C:68:ARG:O	2.21	0.41
1:C:21:GLN:NE2	1:C:41:VAL:H	2.19	0.41
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.55	0.41
1:A:479:TRP:CZ3	1:A:481:GLY:HA2	2.56	0.41
1:E:694:GLN:HB2	1:E:697:HIS:CD2	2.56	0.41
1:E:208:VAL:HA	1:E:240:PHE:O	2.22	0.41
1:A:735:THR:HG23	6:A:3229:HOH:O	2.22	0.40
1:A:689:HIS:ND1	1:A:739:ARG:HD3	2.36	0.40
1:E:376:GLN:HA	1:E:384:LEU:O	2.21	0.40
1:D:608:TYR:CZ	1:D:616:VAL:HG22	2.56	0.40
1:F:744:VAL:HG22	1:F:771:THR:O	2.21	0.40
1:D:735:THR:HG23	6:D:3161:HOH:O	2.21	0.40
1:F:107:ASN:ND2	1:F:125:ASN:HD21	2.20	0.40
1:C:21:GLN:HE22	1:C:41:VAL:H	1.68	0.40
1:D:315:TRP:H	1:D:381:GLN:NE2	2.19	0.40
1:E:315:TRP:N	1:E:381:GLN:HE21	2.17	0.40
1:B:689:HIS:HB3	1:B:739:ARG:HH11	1.86	0.40
1:E:91:LYS:HE2	6:E:3177:HOH:O	2.22	0.40
1:D:80:PRO:HD3	1:D:431:SER:HB3	2.03	0.40
1:A:726:THR:HA	1:A:766:ASN:HD21	1.87	0.40
1:E:652:GLN:NE2	1:E:654:HIS:NE2	2.70	0.40

There are no symmetry-related clashes.

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	771/773 (100%)	744 (96%)	25 (3%)	2 (0%)	46	35
1	B	771/773 (100%)	736 (96%)	33 (4%)	2 (0%)	46	35
1	C	771/773 (100%)	740 (96%)	30 (4%)	1 (0%)	56	48
1	D	771/773 (100%)	743 (96%)	28 (4%)	0	100	100
1	E	771/773 (100%)	740 (96%)	27 (4%)	4 (0%)	34	21
1	F	771/773 (100%)	737 (96%)	28 (4%)	6 (1%)	24	11
All	All	4626/4638 (100%)	4440 (96%)	171 (4%)	15 (0%)	46	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	LEU
1	B	768	LEU
1	E	316	CYS
1	E	477	VAL
1	F	316	CYS
1	B	767	ALA
1	E	766	ASN
1	F	768	LEU
1	C	279	THR
1	E	768	LEU
1	F	77	ASN
1	F	477	VAL
1	F	767	ALA
1	A	348	PRO
1	F	476	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	660/660 (100%)	617 (94%)	43 (6%)	21	8
1	B	660/660 (100%)	618 (94%)	42 (6%)	22	8
1	C	660/660 (100%)	614 (93%)	46 (7%)	19	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	660/660 (100%)	610 (92%)	50 (8%)	16	5
1	E	660/660 (100%)	609 (92%)	51 (8%)	16	5
1	F	660/660 (100%)	617 (94%)	43 (6%)	21	8
All	All	3960/3960 (100%)	3685 (93%)	275 (7%)	19	7

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	48	LEU
1	A	52	LEU
1	A	84	LEU
1	A	120	LEU
1	A	123	LEU
1	A	137	ASN
1	A	174	ARG
1	A	178	THR
1	A	208	VAL
1	A	281	TYR
1	A	300	LEU
1	A	332	ILE
1	A	336	LYS
1	A	347	ASN
1	A	377	TRP
1	A	452	LEU
1	A	459	GLU
1	A	518	THR
1	A	532	LEU
1	A	533	LEU
1	A	573	LEU
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	647	SER
1	A	657	LEU
1	A	671	LEU
1	A	681	VAL
1	A	693	LEU
1	A	714	LEU
1	A	719	THR
1	A	723	ILE

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Mol	Chain	Res	Type
1	A	732	LYS
1	A	735	THR
1	A	736	LEU
1	A	744	VAL
1	A	756	GLU
1	A	757	GLN
1	A	759	LEU
1	A	764	GLN
1	A	768	LEU
1	A	770	ILE
1	B	48	LEU
1	B	84	LEU
1	B	99	ARG
1	B	120	LEU
1	B	137	ASN
1	B	174	ARG
1	B	178	THR
1	B	179	VAL
1	B	208	VAL
1	B	260	ARG
1	B	273	LEU
1	B	347	ASN
1	B	377	TRP
1	B	425	VAL
1	B	452	LEU
1	B	459	GLU
1	B	518	THR
1	B	532	LEU
1	B	533	LEU
1	B	537	SER
1	B	546	ARG
1	B	553	ASP
1	B	573	LEU
1	B	579	ARG
1	B	592	MET
1	B	616	VAL
1	B	630	LEU
1	B	657	LEU
1	B	686	THR
1	B	693	LEU
1	B	714	LEU
1	B	723	ILE

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Mol	Chain	Res	Type
1	B	732	LYS
1	B	735	THR
1	B	736	LEU
1	B	739	ARG
1	B	744	VAL
1	B	747	LEU
1	B	764	GLN
1	B	766	ASN
1	B	771	THR
1	B	773	HIS
1	C	30	ASN
1	C	48	LEU
1	C	52	LEU
1	C	84	LEU
1	C	95	GLU
1	C	120	LEU
1	C	137	ASN
1	C	143	THR
1	C	174	ARG
1	C	178	THR
1	C	179	VAL
1	C	208	VAL
1	C	214	GLN
1	C	264	PRO
1	C	273	LEU
1	C	280	ASN
1	C	281	TYR
1	C	288	SER
1	C	300	LEU
1	C	336	LYS
1	C	347	ASN
1	C	377	TRP
1	C	452	LEU
1	C	453	LYS
1	C	459	GLU
1	C	533	LEU
1	C	573	LEU
1	C	592	MET
1	C	614	VAL
1	C	616	VAL
1	C	630	LEU
1	C	657	LEU

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Mol	Chain	Res	Type
1	C	669	LEU
1	C	671	LEU
1	C	681	VAL
1	C	693	LEU
1	C	714	LEU
1	C	723	ILE
1	C	726	THR
1	C	732	LYS
1	C	736	LEU
1	C	745	ASN
1	C	749	ASP
1	C	756	GLU
1	C	770	ILE
1	C	773	HIS
1	D	45	THR
1	D	48	LEU
1	D	52	LEU
1	D	69	ILE
1	D	84	LEU
1	D	93	THR
1	D	99	ARG
1	D	120	LEU
1	D	137	ASN
1	D	143	THR
1	D	146	GLN
1	D	174	ARG
1	D	178	THR
1	D	208	VAL
1	D	246	THR
1	D	273	LEU
1	D	281	TYR
1	D	300	LEU
1	D	332	ILE
1	D	347	ASN
1	D	377	TRP
1	D	452	LEU
1	D	459	GLU
1	D	518	THR
1	D	532	LEU
1	D	533	LEU
1	D	542	SER
1	D	573	LEU

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Mol	Chain	Res	Type
1	D	592	MET
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	632	GLU
1	D	657	LEU
1	D	671	LEU
1	D	693	LEU
1	D	714	LEU
1	D	723	ILE
1	D	732	LYS
1	D	733	ASN
1	D	735	THR
1	D	736	LEU
1	D	742	VAL
1	D	745	ASN
1	D	755	SER
1	D	764	GLN
1	D	768	LEU
1	D	771	THR
1	D	772	LEU
1	D	773	HIS
1	E	29	ASP
1	E	44	ARG
1	E	52	LEU
1	E	69	ILE
1	E	98	GLU
1	E	99	ARG
1	E	120	LEU
1	E	123	LEU
1	E	137	ASN
1	E	143	THR
1	E	146	GLN
1	E	174	ARG
1	E	178	THR
1	E	208	VAL
1	E	246	THR
1	E	273	LEU
1	E	276	SER
1	E	300	LEU
1	E	316	CYS
1	E	324	THR

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Mol	Chain	Res	Type
1	E	332	ILE
1	E	334	ARG
1	E	347	ASN
1	E	377	TRP
1	E	408	MET
1	E	419	GLU
1	E	425	VAL
1	E	452	LEU
1	E	459	GLU
1	E	477	VAL
1	E	533	LEU
1	E	542	SER
1	E	573	LEU
1	E	616	VAL
1	E	630	LEU
1	E	653	GLN
1	E	657	LEU
1	E	664	ARG
1	E	671	LEU
1	E	693	LEU
1	E	714	LEU
1	E	719	THR
1	E	723	ILE
1	E	736	LEU
1	E	739	ARG
1	E	742	VAL
1	E	764	GLN
1	E	769	THR
1	E	771	THR
1	E	772	LEU
1	E	773	HIS
1	F	44	ARG
1	F	45	THR
1	F	52	LEU
1	F	84	LEU
1	F	95	GLU
1	F	120	LEU
1	F	137	ASN
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	179	VAL

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Mol	Chain	Res	Type
1	F	214	GLN
1	F	273	LEU
1	F	280	ASN
1	F	300	LEU
1	F	316	CYS
1	F	336	LYS
1	F	347	ASN
1	F	377	TRP
1	F	452	LEU
1	F	459	GLU
1	F	492	GLU
1	F	532	LEU
1	F	533	LEU
1	F	537	SER
1	F	544	SER
1	F	573	LEU
1	F	579	ARG
1	F	592	MET
1	F	616	VAL
1	F	630	LEU
1	F	671	LEU
1	F	681	VAL
1	F	693	LEU
1	F	714	LEU
1	F	732	LYS
1	F	735	THR
1	F	736	LEU
1	F	739	ARG
1	F	747	LEU
1	F	764	GLN
1	F	770	ILE
1	F	771	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	27	GLN
1	A	73	GLN
1	A	107	ASN
1	A	125	ASN
1	A	133	GLN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	141	GLN
1	A	212	HIS
1	A	347	ASN
1	A	352	GLN
1	A	381	GLN
1	A	564	GLN
1	A	641	ASN
1	A	652	GLN
1	A	692	ASN
1	A	766	ASN
1	B	21	GLN
1	B	27	GLN
1	B	73	GLN
1	B	107	ASN
1	B	133	GLN
1	B	137	ASN
1	B	177	GLN
1	B	212	HIS
1	B	347	ASN
1	B	352	GLN
1	B	381	GLN
1	B	478	HIS
1	B	652	GLN
1	B	692	ASN
1	B	697	HIS
1	B	733	ASN
1	B	766	ASN
1	C	21	GLN
1	C	27	GLN
1	C	30	ASN
1	C	73	GLN
1	C	107	ASN
1	C	133	GLN
1	C	137	ASN
1	C	141	GLN
1	C	177	GLN
1	C	212	HIS
1	C	347	ASN
1	C	352	GLN
1	C	381	GLN
1	C	478	HIS

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Mol	Chain	Res	Type
1	C	517	ASN
1	C	652	GLN
1	C	692	ASN
1	C	733	ASN
1	D	21	GLN
1	D	27	GLN
1	D	73	GLN
1	D	107	ASN
1	D	125	ASN
1	D	133	GLN
1	D	137	ASN
1	D	141	GLN
1	D	146	GLN
1	D	177	GLN
1	D	212	HIS
1	D	347	ASN
1	D	352	GLN
1	D	381	GLN
1	D	564	GLN
1	D	652	GLN
1	D	692	ASN
1	D	766	ASN
1	E	27	GLN
1	E	73	GLN
1	E	107	ASN
1	E	133	GLN
1	E	137	ASN
1	E	212	HIS
1	E	347	ASN
1	E	352	GLN
1	E	381	GLN
1	E	564	GLN
1	E	652	GLN
1	E	653	GLN
1	E	692	ASN
1	E	697	HIS
1	E	745	ASN
1	E	766	ASN
1	F	21	GLN
1	F	27	GLN
1	F	61	GLN
1	F	73	GLN

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Mol	Chain	Res	Type
1	F	107	ASN
1	F	133	GLN
1	F	137	ASN
1	F	177	GLN
1	F	212	HIS
1	F	280	ASN
1	F	347	ASN
1	F	352	GLN
1	F	381	GLN
1	F	478	HIS
1	F	564	GLN
1	F	652	GLN
1	F	697	HIS
1	F	733	ASN
1	F	748	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](#)

35 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	SO4	A	3008	-	4,4,4	0.21	0	6,6,6	0.43	0
4	XTG	A	3015	-	29,32,32	2.66	4 (13%)	42,46,46	3.03	17 (40%)
5	GOL	A	3024	-	5,5,5	0.38	0	5,5,5	0.83	0
5	GOL	A	3028	-	5,5,5	0.31	0	5,5,5	0.66	0
5	GOL	A	3029	-	5,5,5	0.47	0	5,5,5	1.13	1 (20%)
2	SO4	B	3006	-	4,4,4	0.27	0	6,6,6	0.45	0
3	MPO	B	3010	-	12,13,13	0.81	0	15,17,17	1.34	2 (13%)
4	XTG	B	3016	-	29,32,32	2.88	6 (20%)	42,46,46	3.20	13 (30%)
5	GOL	B	3025	-	5,5,5	0.36	0	5,5,5	1.05	0
5	GOL	B	3026	-	5,5,5	0.27	0	5,5,5	0.78	0
2	SO4	C	3005	-	4,4,4	0.22	0	6,6,6	0.49	0
3	MPO	C	3011	-	12,13,13	0.85	0	15,17,17	1.71	4 (26%)
4	XTG	C	3017	-	29,32,32	2.59	3 (10%)	42,46,46	2.55	6 (14%)
5	GOL	C	3023	-	5,5,5	0.51	0	5,5,5	1.42	1 (20%)
5	GOL	C	3027	-	5,5,5	0.53	0	5,5,5	0.76	0
5	GOL	C	3030	-	5,5,5	0.43	0	5,5,5	0.55	0
2	SO4	D	3002	-	4,4,4	0.18	0	6,6,6	0.55	0
3	MPO	D	3012	-	12,13,13	0.86	0	15,17,17	1.60	2 (13%)
4	XTG	D	3018	-	29,32,32	3.65	9 (31%)	42,46,46	3.41	14 (33%)
5	GOL	D	3031	-	5,5,5	0.37	0	5,5,5	0.63	0
5	GOL	D	3032	-	5,5,5	0.41	0	5,5,5	0.90	0
2	SO4	E	3004	-	4,4,4	0.20	0	6,6,6	0.45	0
2	SO4	E	3009	-	4,4,4	0.29	0	6,6,6	0.43	0
3	MPO	E	3013	-	12,13,13	0.61	0	15,17,17	2.36	2 (13%)
4	XTG	E	3019	-	29,32,32	2.32	5 (17%)	42,46,46	2.60	10 (23%)
5	GOL	E	3033	-	5,5,5	0.37	0	5,5,5	0.63	0
5	GOL	E	3035	-	5,5,5	0.60	0	5,5,5	0.78	0
2	SO4	F	3001	-	4,4,4	0.15	0	6,6,6	0.56	0
2	SO4	F	3003	-	4,4,4	0.55	0	6,6,6	0.23	0
2	SO4	F	3007	-	4,4,4	0.22	0	6,6,6	0.19	0
3	MPO	F	3014	-	12,13,13	8.22	1 (8%)	15,17,17	9.35	6 (40%)
4	XTG	F	3020	-	29,32,32	2.51	8 (27%)	42,46,46	3.01	13 (30%)
4	XTG	F	3021	-	29,32,32	2.58	5 (17%)	42,46,46	2.62	8 (19%)
5	GOL	F	3022	-	5,5,5	0.60	0	5,5,5	0.78	0
5	GOL	F	3034	-	5,5,5	0.39	0	5,5,5	0.48	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	SO4	A	3008	-	-	0/0/0/0	0/0/0/0
4	XTG	A	3015	-	-	0/13/50/50	0/3/3/3
5	GOL	A	3024	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3028	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3029	-	-	0/4/4/4	0/0/0/0
2	SO4	B	3006	-	-	0/0/0/0	0/0/0/0
3	MPO	B	3010	-	-	0/7/15/15	0/1/1/1
4	XTG	B	3016	-	-	0/13/50/50	0/3/3/3
5	GOL	B	3025	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3026	-	-	0/4/4/4	0/0/0/0
2	SO4	C	3005	-	-	0/0/0/0	0/0/0/0
3	MPO	C	3011	-	-	0/7/15/15	0/1/1/1
4	XTG	C	3017	-	-	0/13/50/50	0/3/3/3
5	GOL	C	3023	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3027	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3030	-	-	0/4/4/4	0/0/0/0
2	SO4	D	3002	-	-	0/0/0/0	0/0/0/0
3	MPO	D	3012	-	-	0/7/15/15	0/1/1/1
4	XTG	D	3018	-	-	2/13/50/50	0/3/3/3
5	GOL	D	3031	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3032	-	-	0/4/4/4	0/0/0/0
2	SO4	E	3004	-	-	0/0/0/0	0/0/0/0
2	SO4	E	3009	-	-	0/0/0/0	0/0/0/0
3	MPO	E	3013	-	-	0/7/15/15	0/1/1/1
4	XTG	E	3019	-	-	0/13/50/50	0/3/3/3
5	GOL	E	3033	-	-	0/4/4/4	0/0/0/0
5	GOL	E	3035	-	-	0/4/4/4	0/0/0/0
2	SO4	F	3001	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3003	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3007	-	-	0/0/0/0	0/0/0/0
3	MPO	F	3014	-	-	0/7/15/15	0/1/1/1
4	XTG	F	3020	-	-	0/13/50/50	0/3/3/3
4	XTG	F	3021	-	-	0/13/50/50	0/3/3/3
5	GOL	F	3022	-	-	0/4/4/4	0/0/0/0
5	GOL	F	3034	-	-	0/4/4/4	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3019	XTG	O5-C1	2.00	1.47	1.41
4	C	3017	XTG	C8-C9	2.15	1.58	1.52
4	A	3015	XTG	C10-C9	2.15	1.55	1.52
4	F	3020	XTG	O7-C9	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3020	XTG	O9-C7	2.24	1.46	1.41
4	D	3018	XTG	O6-C8	2.26	1.48	1.43
4	D	3018	XTG	C10-C9	2.30	1.55	1.52
4	B	3016	XTG	O9-C11	2.34	1.47	1.43
4	F	3020	XTG	O5-C1	2.47	1.48	1.41
4	F	3020	XTG	C8-C9	2.50	1.59	1.52
4	F	3021	XTG	C7-S6	2.82	1.85	1.80
4	F	3020	XTG	O6-C8	2.89	1.49	1.43
4	F	3021	XTG	C11-C10	2.94	1.59	1.52
4	C	3017	XTG	C7-S6	2.95	1.85	1.80
4	B	3016	XTG	C8-C9	3.07	1.60	1.52
4	E	3019	XTG	O1-C1	3.17	1.46	1.41
4	E	3019	XTG	C10-C9	3.39	1.57	1.52
4	D	3018	XTG	C8-C9	3.84	1.62	1.52
4	F	3020	XTG	C10-C9	3.86	1.57	1.52
4	B	3016	XTG	C7-S6	4.14	1.87	1.80
4	A	3015	XTG	O1-C1	4.29	1.48	1.41
4	F	3021	XTG	O9-C7	4.29	1.51	1.41
4	A	3015	XTG	C7-S6	4.37	1.87	1.80
4	D	3018	XTG	C7-C8	4.52	1.61	1.53
4	B	3016	XTG	C10-C9	4.52	1.58	1.52
4	E	3019	XTG	C7-S6	4.66	1.88	1.80
4	F	3021	XTG	O9-C11	4.84	1.51	1.43
4	F	3020	XTG	C7-S6	5.26	1.89	1.80
4	D	3018	XTG	O8-C10	5.46	1.55	1.43
4	D	3018	XTG	O9-C7	5.77	1.54	1.41
4	B	3016	XTG	O1-C1	5.82	1.50	1.41
4	D	3018	XTG	C7-S6	6.08	1.90	1.80
4	D	3018	XTG	O9-C11	7.14	1.55	1.43
4	E	3019	XTG	O11-N1	9.14	1.40	1.22
4	F	3020	XTG	O11-N1	9.80	1.42	1.22
4	F	3021	XTG	O11-N1	10.69	1.44	1.22
4	B	3016	XTG	O11-N1	11.31	1.45	1.22
4	A	3015	XTG	O11-N1	11.77	1.46	1.22
4	C	3017	XTG	O11-N1	12.74	1.48	1.22
4	D	3018	XTG	O11-N1	13.20	1.48	1.22
3	F	3014	MPO	C4-N1	28.31	2.24	1.46

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3014	MPO	C7-N1-C4	-14.47	77.56	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3020	XTG	C1-O5-C5	-7.20	99.77	113.75
4	D	3018	XTG	C11-C10-C9	-6.93	101.35	109.54
4	F	3020	XTG	C6-C5-C4	-6.12	98.07	112.88
4	B	3016	XTG	C15-O1-C1	-5.92	109.04	117.87
4	E	3019	XTG	O9-C7-C8	-5.92	102.04	110.14
4	A	3015	XTG	C1-O5-C5	-5.39	103.27	113.75
4	F	3021	XTG	O5-C5-C6	-4.80	99.32	106.60
4	D	3018	XTG	C6-C5-C4	-4.15	102.83	112.88
4	C	3017	XTG	C3-C4-C5	-3.46	104.17	110.20
4	C	3017	XTG	C1-O5-C5	-3.45	107.05	113.75
4	E	3019	XTG	C1-O5-C5	-3.40	107.14	113.75
4	F	3020	XTG	C15-O1-C1	-3.39	112.81	117.87
4	D	3018	XTG	O9-C7-C8	-3.12	105.86	110.14
4	B	3016	XTG	C3-C4-C5	-3.07	104.85	110.20
4	B	3016	XTG	O9-C7-C8	-2.96	106.08	110.14
4	B	3016	XTG	C1-O5-C5	-2.94	108.04	113.75
4	A	3015	XTG	C3-C4-C5	-2.70	105.49	110.20
4	A	3015	XTG	C6-C5-C4	-2.66	106.44	112.88
4	A	3015	XTG	O5-C5-C4	-2.51	104.97	109.68
4	D	3018	XTG	C10-C9-C8	-2.50	106.79	111.04
3	D	3012	MPO	O3-S1-O2	-2.48	105.85	111.61
3	C	3011	MPO	O3-S1-O2	-2.46	105.89	111.61
4	A	3015	XTG	O9-C7-C8	-2.43	106.81	110.14
4	C	3017	XTG	O2-C2-C1	-2.34	104.89	110.02
4	F	3020	XTG	O3-C3-C2	-2.34	105.07	110.34
4	F	3020	XTG	C3-C4-C5	-2.33	106.14	110.20
4	A	3015	XTG	C4-C3-C2	-2.31	106.47	110.79
4	A	3015	XTG	O6-C8-C7	-2.23	106.10	110.43
3	F	3014	MPO	O2-S1-O1	-2.17	105.58	113.48
4	E	3019	XTG	C3-C4-C5	-2.17	106.42	110.20
4	A	3015	XTG	O5-C1-C2	-2.12	105.93	110.28
4	B	3016	XTG	O5-C1-C2	-2.08	106.02	110.28
4	F	3021	XTG	C1-O5-C5	-2.06	109.74	113.75
4	F	3020	XTG	C4-C3-C2	-2.04	106.98	110.79
3	C	3011	MPO	O2-S1-O1	-2.01	106.14	113.48
3	B	3010	MPO	O2-S1-C1	2.01	108.62	106.91
5	A	3029	GOL	O2-C2-C1	2.03	117.97	108.65
4	E	3019	XTG	C15-O1-C1	2.13	121.05	117.87
5	C	3023	GOL	O2-C2-C3	2.16	118.56	108.65
4	E	3019	XTG	O5-C1-O1	2.16	114.16	108.39
4	F	3021	XTG	O8-C10-C11	2.19	113.59	109.21
4	B	3016	XTG	O8-C10-C9	2.23	114.60	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3020	XTG	C17-C12-N1	2.24	121.29	119.48
4	A	3015	XTG	O1-C1-C2	2.26	110.81	107.12
4	B	3016	XTG	C11-C10-C9	2.31	112.27	109.54
4	B	3016	XTG	C13-C12-N1	2.33	121.36	119.48
4	D	3018	XTG	O5-C1-O1	2.43	114.87	108.39
4	E	3019	XTG	O1-C1-C2	2.53	111.23	107.12
4	D	3018	XTG	O9-C7-S6	2.56	116.21	109.84
4	A	3015	XTG	O7-C9-C8	2.58	116.14	110.34
4	A	3015	XTG	C13-C12-N1	2.58	121.57	119.48
4	D	3018	XTG	O6-C8-C7	2.58	115.46	110.43
3	C	3011	MPO	O2-S1-C1	2.62	109.14	106.91
4	F	3020	XTG	O7-C9-C8	2.72	116.45	110.34
4	F	3021	XTG	O9-C7-S6	2.77	116.74	109.84
4	A	3015	XTG	O11-N1-C12	2.84	123.99	118.89
4	E	3019	XTG	C11-C10-C9	2.89	112.96	109.54
4	D	3018	XTG	O7-C9-C8	2.90	116.86	110.34
4	E	3019	XTG	C17-C12-N1	3.01	121.91	119.48
4	F	3020	XTG	O1-C1-C2	3.02	112.05	107.12
3	B	3010	MPO	O1-S1-C1	3.07	109.53	106.91
4	B	3016	XTG	O6-C8-C9	3.19	117.52	110.34
4	A	3015	XTG	O9-C11-C10	3.22	116.07	110.86
4	A	3015	XTG	O5-C1-O1	3.24	117.03	108.39
4	F	3020	XTG	O9-C7-C8	3.30	114.65	110.14
4	F	3020	XTG	O6-C8-C9	3.42	118.03	110.34
4	C	3017	XTG	O9-C11-C10	3.48	116.50	110.86
4	A	3015	XTG	O6-C8-C9	3.59	118.41	110.34
4	E	3019	XTG	O5-C5-C6	3.59	112.04	106.60
4	D	3018	XTG	O6-C8-C9	3.62	118.49	110.34
4	F	3021	XTG	C6-C5-C4	3.64	121.69	112.88
4	B	3016	XTG	O1-C1-C2	4.01	113.65	107.12
4	D	3018	XTG	O8-C10-C9	4.02	118.21	110.12
4	B	3016	XTG	O5-C1-O1	4.32	119.92	108.39
3	C	3011	MPO	O1-S1-C1	4.40	110.66	106.91
4	F	3021	XTG	O9-C7-C8	4.50	116.29	110.14
4	D	3018	XTG	O9-C11-C10	4.57	118.28	110.86
3	D	3012	MPO	O1-S1-C1	4.62	110.84	106.91
3	E	3013	MPO	O2-S1-C1	5.23	111.36	106.91
4	C	3017	XTG	O5-C5-C6	5.37	114.75	106.60
3	F	3014	MPO	C3-N1-C7	5.93	126.46	111.27
3	E	3013	MPO	O1-S1-C1	6.31	112.29	106.91
4	F	3021	XTG	O9-C11-C10	6.56	121.50	110.86
4	D	3018	XTG	O8-C10-C11	6.62	122.47	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3020	XTG	O5-C5-C6	8.82	119.97	106.60
3	F	3014	MPO	O2-S1-C1	9.70	115.18	106.91
4	D	3018	XTG	O5-C5-C6	9.81	121.47	106.60
4	A	3015	XTG	O5-C5-C6	9.89	121.59	106.60
4	F	3020	XTG	C6-S6-C7	10.38	112.31	100.54
3	F	3014	MPO	C5-C4-N1	11.46	127.48	110.12
4	B	3016	XTG	O5-C5-C6	11.70	124.33	106.60
4	F	3021	XTG	C6-S6-C7	11.96	114.11	100.54
4	A	3015	XTG	C6-S6-C7	12.00	114.15	100.54
4	B	3016	XTG	C6-S6-C7	12.30	114.49	100.54
4	E	3019	XTG	C6-S6-C7	12.37	114.58	100.54
4	D	3018	XTG	C6-S6-C7	12.92	115.19	100.54
4	C	3017	XTG	C6-S6-C7	13.15	115.45	100.54
3	F	3014	MPO	C6-C7-N1	28.67	153.57	110.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3018	XTG	C17-C12-N1-O11
4	D	3018	XTG	C13-C12-N1-O11

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3015	XTG	2	0
5	A	3024	GOL	1	0
5	A	3028	GOL	1	0
5	A	3029	GOL	3	0
4	B	3016	XTG	1	0
5	B	3026	GOL	2	0
5	C	3023	GOL	1	0
2	D	3002	SO4	1	0
4	D	3018	XTG	7	0
5	D	3032	GOL	2	0
2	E	3004	SO4	1	0
4	E	3019	XTG	1	0
2	F	3001	SO4	2	0
2	F	3003	SO4	1	0
4	F	3020	XTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3022	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	773/773 (100%)	-0.17	19 (2%) 61 71	8, 14, 35, 53	0
1	B	773/773 (100%)	0.00	23 (2%) 54 64	11, 20, 38, 58	0
1	C	773/773 (100%)	-0.08	16 (2%) 67 75	9, 18, 35, 50	0
1	D	773/773 (100%)	-0.04	27 (3%) 48 58	8, 17, 41, 55	0
1	E	773/773 (100%)	-0.01	22 (2%) 56 66	10, 20, 39, 55	0
1	F	773/773 (100%)	-0.09	16 (2%) 67 75	9, 17, 37, 54	0
All	All	4638/4638 (100%)	-0.06	123 (2%) 58 68	8, 18, 38, 58	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	545	TYR	7.6
1	D	773	HIS	6.0
1	B	765	GLY	6.0
1	B	767	ALA	5.8
1	C	773	HIS	5.4
1	E	766	ASN	5.1
1	E	46	TRP	4.9
1	B	766	ASN	4.7
1	D	517	ASN	4.6
1	B	517	ASN	4.5
1	D	765	GLY	4.4
1	A	768	LEU	4.4
1	F	773	HIS	4.2
1	F	767	ALA	4.1
1	E	767	ALA	4.0
1	E	765	GLY	3.9
1	B	773	HIS	3.9
1	E	773	HIS	3.9
1	A	773	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	517	ASN	3.8
1	F	46	TRP	3.7
1	B	518	THR	3.7
1	E	518	THR	3.6
1	B	764	GLN	3.6
1	F	766	ASN	3.6
1	A	117	PHE	3.5
1	A	765	GLY	3.4
1	A	766	ASN	3.4
1	D	742	VAL	3.4
1	F	765	GLY	3.3
1	A	278	THR	3.3
1	B	543	LYS	3.2
1	C	765	GLY	3.2
1	B	46	TRP	3.2
1	A	517	ASN	3.1
1	D	519	ALA	3.1
1	B	748	GLN	3.0
1	A	745	ASN	3.0
1	B	754	GLU	3.0
1	D	518	THR	2.9
1	F	768	LEU	2.9
1	D	766	ASN	2.9
1	C	744	VAL	2.9
1	D	117	PHE	2.9
1	A	767	ALA	2.9
1	C	720	GLY	2.9
1	D	542	SER	2.9
1	D	764	GLN	2.8
1	D	756	GLU	2.8
1	A	518	THR	2.8
1	D	29	ASP	2.8
1	F	76	LEU	2.8
1	E	43	GLU	2.8
1	E	545	TYR	2.8
1	D	323	LEU	2.7
1	E	117	PHE	2.7
1	D	544	SER	2.7
1	C	127	GLU	2.6
1	F	518	THR	2.6
1	A	748	GLN	2.6
1	D	88	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	281	TYR	2.6
1	F	754	GLU	2.6
1	C	745	ASN	2.6
1	D	484	TYR	2.6
1	B	756	GLU	2.5
1	D	46	TRP	2.5
1	D	745	ASN	2.5
1	D	543	LYS	2.5
1	B	745	ASN	2.5
1	C	117	PHE	2.4
1	A	46	TRP	2.4
1	D	743	LYS	2.4
1	E	721	ASN	2.4
1	C	764	GLN	2.4
1	E	42	ARG	2.4
1	F	517	ASN	2.4
1	C	748	GLN	2.4
1	C	323	LEU	2.4
1	C	766	ASN	2.3
1	B	98	GLU	2.3
1	E	45	THR	2.3
1	D	748	GLN	2.3
1	B	284	ALA	2.3
1	F	323	LEU	2.3
1	B	332	ILE	2.3
1	F	29	ASP	2.3
1	A	280	ASN	2.3
1	B	280	ASN	2.2
1	A	772	LEU	2.2
1	E	89	ASP	2.2
1	C	208	VAL	2.2
1	A	770	ILE	2.2
1	F	756	GLU	2.2
1	E	208	VAL	2.2
1	B	333	ARG	2.2
1	D	98	GLU	2.2
1	A	721	ASN	2.2
1	F	771	THR	2.2
1	B	88	GLN	2.2
1	B	533	LEU	2.2
1	E	543	LYS	2.2
1	D	100	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	551	TYR	2.1
1	C	756	GLU	2.1
1	E	745	ASN	2.1
1	C	88	GLN	2.1
1	C	46	TRP	2.1
1	A	29	ASP	2.1
1	E	764	GLN	2.1
1	F	88	GLN	2.1
1	D	277	PHE	2.1
1	C	634	ARG	2.1
1	A	323	LEU	2.1
1	E	76	LEU	2.1
1	B	99	ARG	2.1
1	B	759	LEU	2.1
1	E	323	LEU	2.1
1	D	67	VAL	2.0
1	F	117	PHE	2.0
1	A	742	VAL	2.0
1	E	99	ARG	2.0
1	B	346	ILE	2.0

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	MPO	F	3014	13/13	0.76	0.27	9.50	41,62,71,72	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	E	3009	5/5	0.90	0.26	7.79	68,68,69,69	0
5	GOL	A	3029	6/6	0.82	0.24	7.26	30,39,39,39	0
5	GOL	B	3026	6/6	0.90	0.21	5.16	34,39,40,41	0
4	XTG	F	3021	30/30	0.92	0.16	4.76	12,18,54,56	0
3	MPO	D	3012	13/13	0.96	0.15	3.40	20,34,40,40	0
3	MPO	E	3013	13/13	0.95	0.16	2.87	43,49,55,56	0
5	GOL	D	3032	6/6	0.90	0.16	2.74	31,37,40,41	0
5	GOL	A	3024	6/6	0.87	0.25	2.14	37,40,40,40	0
3	MPO	B	3010	13/13	0.97	0.14	1.97	29,36,43,43	0
5	GOL	C	3023	6/6	0.92	0.12	1.49	25,29,29,30	0
5	GOL	E	3035	6/6	0.77	0.19	1.48	54,55,56,56	0
3	MPO	C	3011	13/13	0.95	0.16	1.42	29,34,37,38	0
5	GOL	C	3027	6/6	0.88	0.16	1.25	41,44,45,45	0
4	XTG	D	3018	30/30	0.79	0.20	1.08	24,45,53,56	0
4	XTG	F	3020	30/30	0.92	0.14	0.40	12,38,41,44	0
4	XTG	C	3017	30/30	0.94	0.13	0.20	12,26,39,43	0
4	XTG	E	3019	30/30	0.92	0.13	0.14	17,28,42,47	0
4	XTG	A	3015	30/30	0.94	0.12	0.00	12,28,37,40	0
5	GOL	F	3022	6/6	0.97	0.08	-0.06	16,18,20,22	0
4	XTG	B	3016	30/30	0.93	0.11	-0.32	12,32,41,44	0
2	SO4	F	3003	5/5	0.99	0.08	-0.92	14,16,20,20	0
5	GOL	B	3025	6/6	0.92	0.15	-	26,31,31,32	0
2	SO4	F	3007	5/5	0.97	0.19	-	48,49,50,50	0
5	GOL	D	3031	6/6	0.89	0.13	-	23,28,30,32	0
2	SO4	E	3004	5/5	0.94	0.26	-	45,47,48,49	0
2	SO4	A	3008	5/5	0.94	0.24	-	45,46,48,49	0
5	GOL	A	3028	6/6	0.85	0.20	-	29,35,37,39	0
5	GOL	F	3034	6/6	0.90	0.16	-	32,37,38,38	0
5	GOL	E	3033	6/6	0.86	0.14	-	29,34,35,37	0
2	SO4	F	3001	5/5	0.95	0.20	-	37,39,41,44	0
2	SO4	C	3005	5/5	0.96	0.21	-	46,48,49,50	0
2	SO4	D	3002	5/5	0.96	0.23	-	51,52,53,54	0
5	GOL	C	3030	6/6	0.91	0.14	-	25,28,30,30	0
2	SO4	B	3006	5/5	0.95	0.24	-	45,47,49,50	0

6.5 Other polymers

There are no such residues in this entry.