Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:42 PM GMT

PDB ID	:	4D0Z
Title	:	GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 and manganese (Higher resolution dataset)
Authors	:	Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on	:	2014-04-30
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

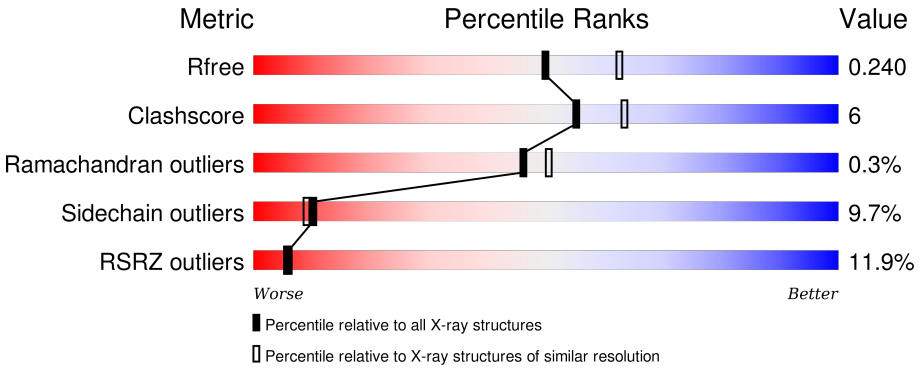
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	571	3% 71% 13% • 13%
1	B	571	3% 73% 12% • 13%
1	C	571	35% 64% 15% • • 17%
1	D	571	3% 70% 14% • 13%
1	E	571	2% 71% 12% • 13%

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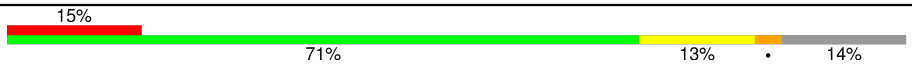
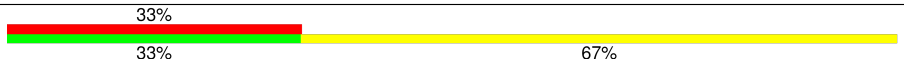
Mol	Chain	Length	Quality of chain
1	F	571	
2	X	6	
2	Y	6	

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
4	EDO	A	1572	-	-	X	-
4	EDO	A	1573	-	-	-	X
4	EDO	A	1574	-	-	-	X
4	EDO	A	1576	-	-	-	X
4	EDO	A	1577	-	-	-	X
4	EDO	A	1579	-	-	-	X
4	EDO	A	1580	-	-	-	X
4	EDO	B	1573	-	-	X	X
4	EDO	B	1578	-	-	-	X
4	EDO	D	1576	-	-	X	-
4	EDO	E	1570	-	-	-	X
4	EDO	E	1572	-	-	X	-
4	EDO	E	1577	-	-	-	X
5	BBK	B	1580	-	-	-	X
5	BBK	D	1572	-	-	-	X
5	BBK	E	1584	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24773 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 POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	20	1	0
			3975	2502	722	727	24			
1	B	495	Total	C	N	O	S	20	0	0
			3967	2497	719	727	24			
1	C	476	Total	C	N	O	S	20	0	0
			3826	2407	693	702	24			
1	D	495	Total	C	N	O	S	20	0	0
			3967	2497	719	727	24			
1	E	495	Total	C	N	O	S	20	0	0
			3967	2497	719	727	24			
1	F	491	Total	C	N	O	S	20	0	0
			3926	2470	710	722	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
B	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
C	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
D	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
E	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
F	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471

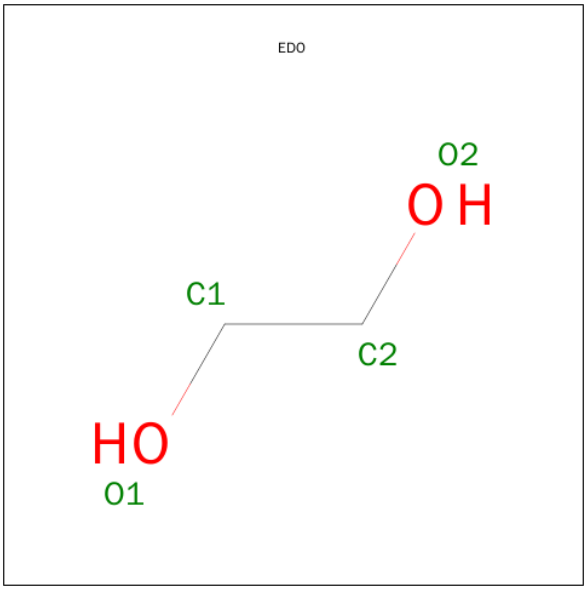
- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
2	Y	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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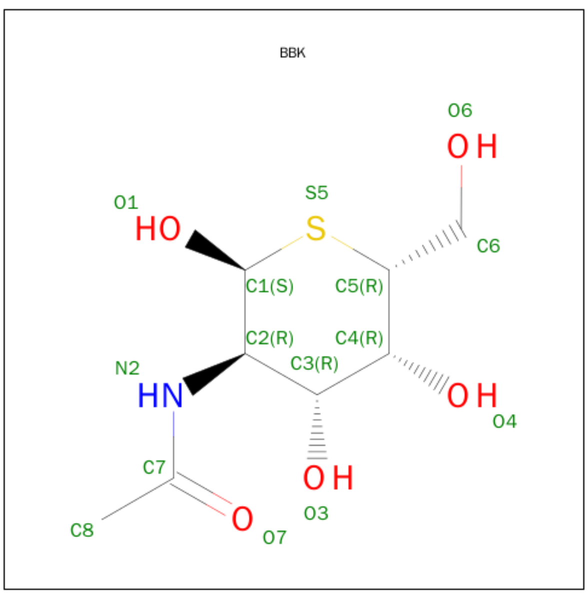
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-5-THIO-ALPHA-D-GALACTOPYRANOSE) (three-letter code: BBK) (formula: $C_8H_{15}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 15	C 8	N 1	O 5	S 1	0	0

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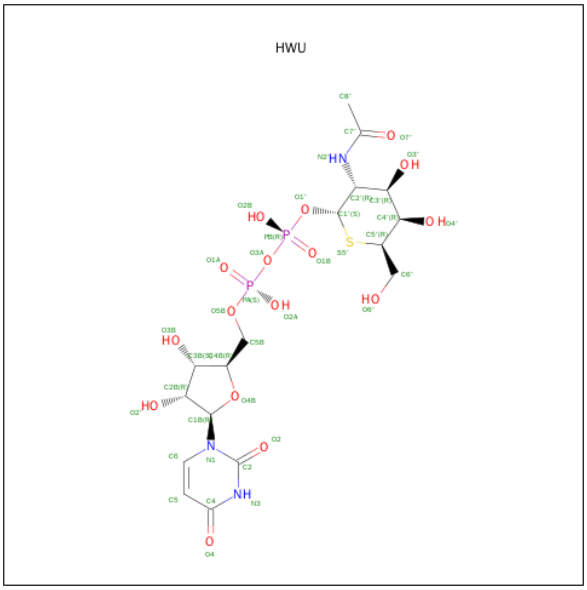
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 6 is (2R,3R,4R,5R,6R)-3-(ACETYLAMINO)-4,5-DIHYDROXY-6-(HYDROXYMETHYL)TETRAHYDRO-2H-THIOPYRAN-2-YL [(2R,3S,4R,5R)-5-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: HWU) (formula: $C_{17}H_{27}N_3O_{16}P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	D	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	E	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	F	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

- Molecule 7 is water.

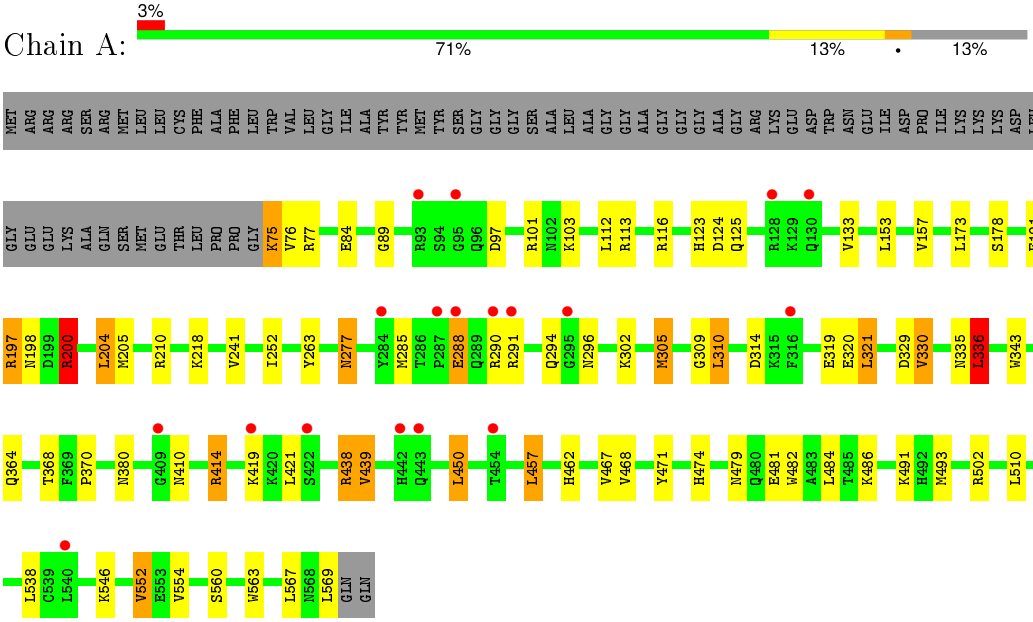
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	144	Total O 144 144	0	0
7	B	125	Total O 125 125	0	0
7	C	13	Total O 13 13	0	0
7	D	122	Total O 122 122	0	0
7	E	168	Total O 168 168	0	0
7	F	61	Total O 61 61	0	0

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.

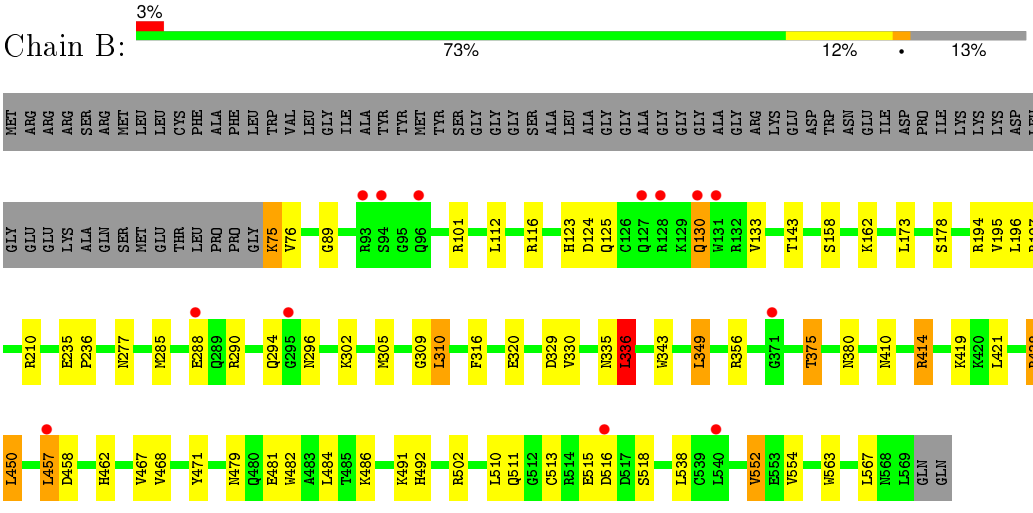
- Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain A:



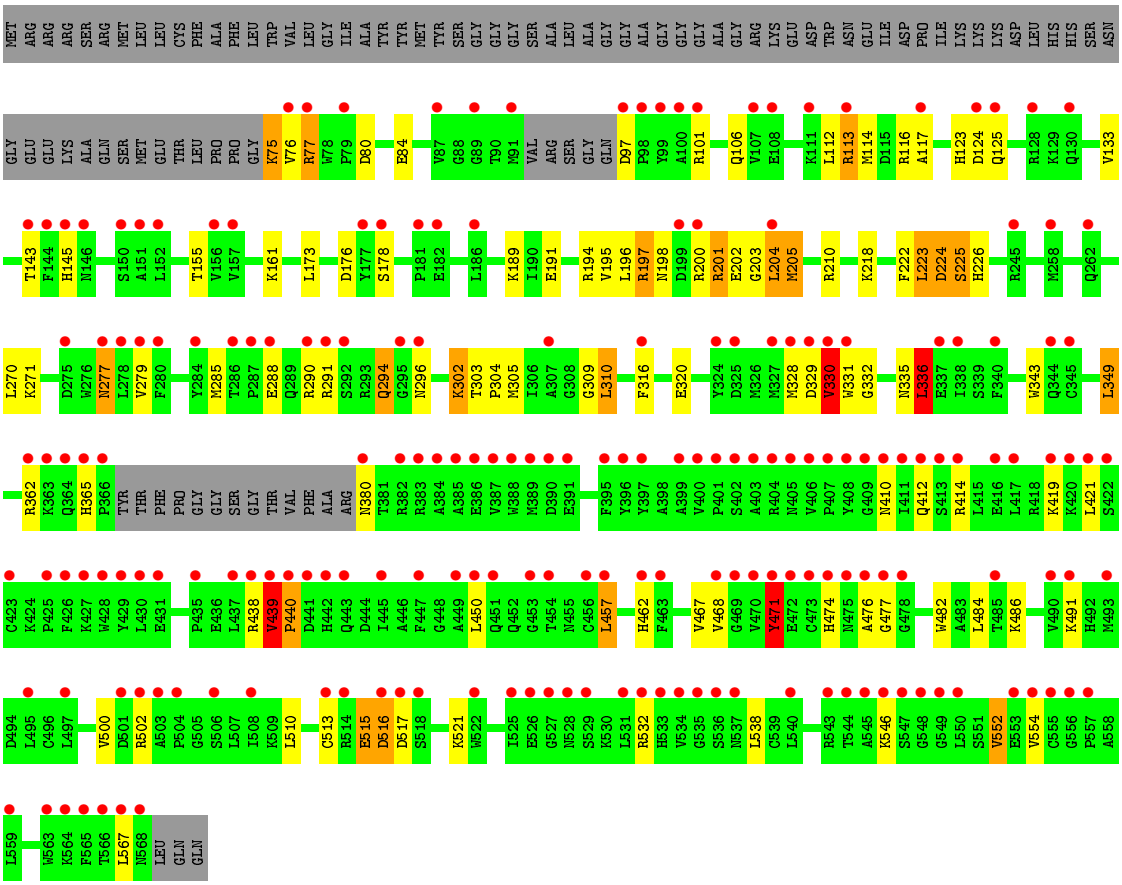
- Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain B:



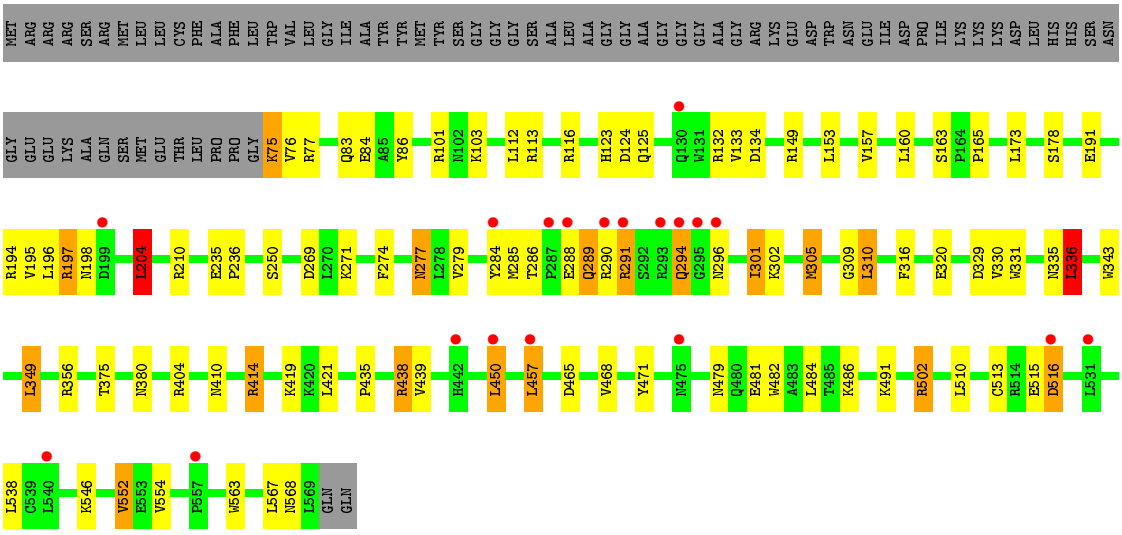
- Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain C:



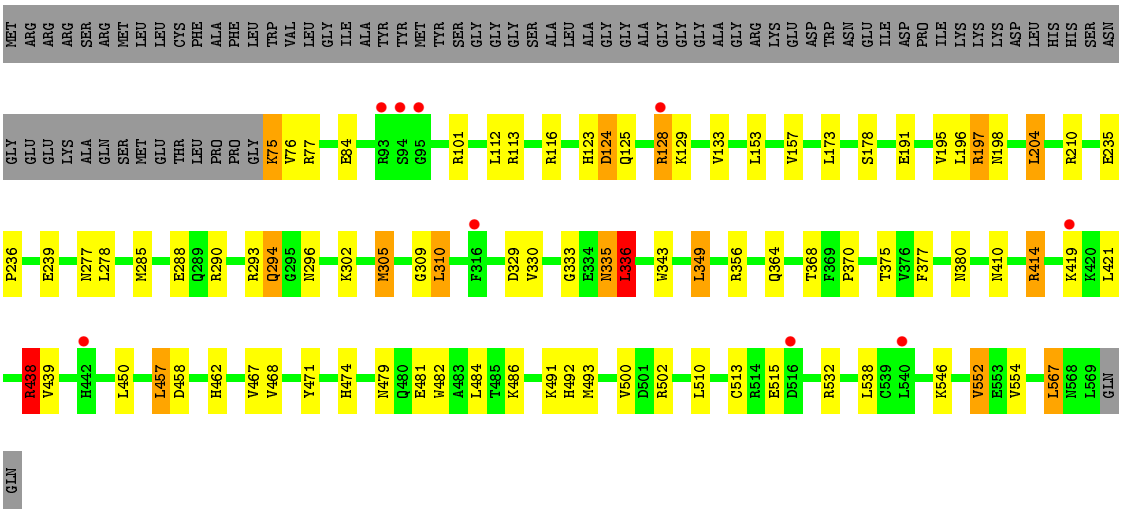
• Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain D:



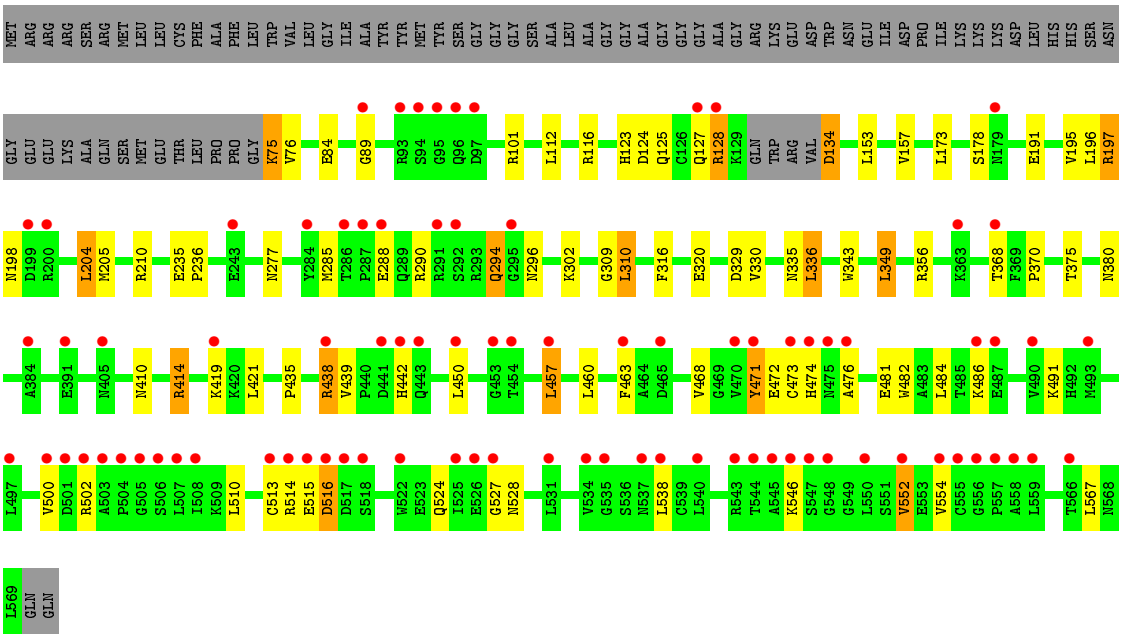
• Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain E:



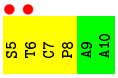
• Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain F:



• Molecule 2: PEPTIDE

Chain X:



• Molecule 2: PEPTIDE

Chain Y:


S5
T6
C7
P8
A9
A10

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.48Å 121.14Å 249.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.39 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (249.39-2.20) 99.8 (19.95-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.196 , 0.234 0.204 , 0.240	Depositor DCC
R_{free} test set	4937 reflections (2.85%)	DCC
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.1	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 178449 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24773	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: HWU, BBK, EDO, MN

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	0.85	4/4070 (0.1%)	0.98	25/5503 (0.5%)
1	B	0.79	3/4059 (0.1%)	0.91	9/5489 (0.2%)
1	C	0.88	7/3912 (0.2%)	0.98	26/5287 (0.5%)
1	D	1.01	3/4059 (0.1%)	0.98	19/5489 (0.3%)
1	E	0.92	3/4059 (0.1%)	0.98	19/5489 (0.3%)
1	F	0.89	3/4015 (0.1%)	0.90	12/5427 (0.2%)
2	X	1.42	0/32	1.09	0/44
2	Y	1.82	1/32 (3.1%)	1.53	0/44
All	All	0.89	24/24238 (0.1%)	0.95	110/32772 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	LYS	CB-CG	-33.78	0.61	1.52
1	C	84	GLU	CB-CG	-26.41	1.01	1.52
1	D	486	LYS	CB-CG	-25.36	0.84	1.52
1	F	75	LYS	CB-CG	-25.00	0.85	1.52
1	E	84	GLU	CB-CG	-23.77	1.06	1.52
1	F	84	GLU	CB-CG	-23.05	1.08	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	486	LYS	CB-CG	-20.62	0.96	1.52
1	C	224	ASP	C-N	-20.14	0.87	1.34
1	A	84	GLU	CB-CG	-16.34	1.21	1.52
1	A	75	LYS	CB-CG	-14.91	1.12	1.52
1	C	225	SER	C-N	-14.91	0.99	1.34
1	E	75	LYS	CB-CG	-14.21	1.14	1.52
1	C	222	PHE	C-N	12.92	1.63	1.34
1	B	75	LYS	CB-CG	-12.78	1.18	1.52
1	A	486	LYS	CB-CG	-10.92	1.23	1.52
1	C	486	LYS	CB-CG	-10.47	1.24	1.52
1	B	515	GLU	CB-CG	-9.63	1.33	1.52
1	C	223	LEU	C-N	7.13	1.50	1.34
1	C	75	LYS	CB-CG	-6.90	1.33	1.52
2	Y	9	ALA	C-O	6.73	1.36	1.23
1	B	294	GLN	CB-CG	6.40	1.69	1.52
1	A	294	GLN	CB-CG	5.63	1.67	1.52
1	E	294	GLN	CB-CG	5.50	1.67	1.52
1	D	250	SER	CB-OG	-5.18	1.35	1.42

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	LYS	CA-CB-CG	21.27	160.19	113.40
1	D	194	ARG	NE-CZ-NH2	-17.68	111.46	120.30
1	E	75	LYS	CA-CB-CG	16.43	149.55	113.40
1	F	75	LYS	CA-CB-CG	15.46	147.41	113.40
1	D	75	LYS	CB-CG-CD	13.48	146.66	111.60
1	E	486	LYS	CB-CG-CD	-12.84	78.21	111.60
1	C	75	LYS	CA-CB-CG	12.77	141.48	113.40
1	B	486	LYS	CB-CG-CD	-11.69	81.22	111.60
1	F	84	GLU	CA-CB-CG	11.10	137.83	113.40
1	A	200	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	D	75	LYS	CA-CB-CG	10.92	137.41	113.40
1	C	225	SER	O-C-N	-10.49	105.92	122.70
1	D	194	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	E	84	GLU	CA-CB-CG	10.22	135.89	113.40
1	D	204	LEU	CA-CB-CG	9.38	136.88	115.30
1	C	225	SER	CA-C-N	9.35	137.77	117.20
1	B	486	LYS	CA-CB-CG	-9.22	93.12	113.40
1	C	567	LEU	CA-CB-CG	9.10	136.22	115.30
1	E	486	LYS	CA-CB-CG	-9.09	93.40	113.40
1	A	486	LYS	CB-CG-CD	-9.09	87.98	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294	GLN	CB-CG-CD	8.58	133.90	111.60
1	A	84	GLU	CA-CB-CG	8.46	132.02	113.40
1	C	223	LEU	O-C-N	-8.39	109.28	122.70
1	B	204	LEU	CA-CB-CG	8.37	134.54	115.30
1	C	471	TYR	CA-CB-CG	8.19	128.96	113.40
1	C	84	GLU	CA-CB-CG	8.12	131.27	113.40
1	E	204	LEU	CA-CB-CG	8.07	133.86	115.30
1	D	414	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	294	GLN	CA-CB-CG	-7.93	95.96	113.40
1	C	225	SER	N-CA-C	-7.82	89.90	111.00
1	A	321	LEU	N-CA-C	-7.78	90.00	111.00
1	E	128	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	225	SER	C-N-CA	7.48	140.40	121.70
1	B	414	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	D	404	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	414	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	E	129	LYS	CD-CE-NZ	7.32	128.55	111.70
1	D	414	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	E	414	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	D	294	GLN	CB-CG-CD	6.98	129.75	111.60
1	E	532	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	113	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	F	527	GLY	N-CA-C	-6.88	95.89	113.10
1	A	197	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	414	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	414	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	567	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	200	ARG	CD-NE-CZ	6.52	132.73	123.60
1	F	294	GLN	CA-CB-CG	-6.50	99.10	113.40
1	C	439	VAL	CB-CA-C	6.48	123.71	111.40
1	B	414	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	E	294	GLN	CB-CG-CD	6.41	128.28	111.60
1	F	356	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	F	414	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	302	LYS	N-CA-C	6.33	128.09	111.00
1	C	223	LEU	C-N-CA	6.30	137.46	121.70
1	A	197	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	194[A]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	194[B]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	356	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	194	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	314	ASP	CB-CG-OD2	-6.05	112.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	197	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	330	VAL	CA-CB-CG2	-6.01	101.89	110.90
1	A	486	LYS	CA-CB-CG	-5.99	100.22	113.40
1	E	336	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	103	LYS	CD-CE-NZ	5.91	125.30	111.70
1	E	414	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	E	197	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	336	LEU	CA-CB-CG	5.85	128.75	115.30
1	F	336	LEU	CA-CB-CG	5.84	128.74	115.30
1	E	532	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	356	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	294	GLN	CA-CB-CG	-5.75	100.75	113.40
1	A	97	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	305	MET	CG-SD-CE	-5.68	91.11	100.20
1	F	567	LEU	CA-CB-CG	5.62	128.23	115.30
1	C	336	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	336	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	321	LEU	CA-C-N	5.57	127.33	116.20
1	E	356	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	414	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	D	404	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	75	LYS	CA-CB-CG	5.50	125.49	113.40
1	D	197	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	336	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	194[A]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	194[B]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	77	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	362	ARG	CG-CD-NE	5.38	123.11	111.80
1	E	84	GLU	CB-CG-CD	5.38	128.74	114.20
1	C	97	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	197	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	197	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	F	486	LYS	CA-CB-CG	5.28	125.02	113.40
1	C	532	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	567	LEU	CA-CB-CG	5.25	127.38	115.30
1	E	438	ARG	CB-CG-CD	5.25	125.25	111.60
1	E	305	MET	CG-SD-CE	-5.24	91.81	100.20
1	C	477	GLY	N-CA-C	5.23	126.18	113.10
1	D	305	MET	CG-SD-CE	-5.22	91.85	100.20
1	C	218	LYS	CB-CA-C	-5.18	100.03	110.40
1	B	356	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	113	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	194	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	356	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	569	LEU	CB-CG-CD2	5.09	119.66	111.00
1	C	194	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	218	LYS	CB-CA-C	-5.07	100.27	110.40
1	D	113	ARG	N-CA-CB	-5.03	101.54	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	GLY	Peptide
1	B	89	GLY	Peptide
1	C	223	LEU	Mainchain
1	F	89	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3975	0	3903	54	0
1	B	3967	0	3890	30	0
1	C	3826	0	3748	81	0
1	D	3967	0	3890	55	0
1	E	3967	0	3890	49	0
1	F	3926	0	3849	31	0
2	X	32	0	28	3	0
2	Y	32	0	28	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	40	0	60	9	0
4	B	32	0	48	6	0
4	D	20	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	56	0	84	15	0
5	A	15	0	15	3	0
5	B	15	0	14	4	0
5	D	15	0	14	4	0
5	E	15	0	13	5	0
6	A	39	0	24	0	0
6	B	39	0	24	2	0
6	C	39	0	25	11	0
6	D	39	0	25	4	0
6	E	39	0	25	2	0
6	F	39	0	24	2	0
7	A	144	0	0	0	0
7	B	125	0	0	3	0
7	C	13	0	0	6	0
7	D	122	0	0	3	0
7	E	168	0	0	3	0
7	F	61	0	0	0	0
All	All	24773	0	23651	298	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 6.

All (298) 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:C:203:GLY:HA3	1:C:330:VAL:CG2	1.71	1.19
1:C:203:GLY:CA	1:C:330:VAL:CG2	2.26	1.13
1:A:291:ARG:CZ	1:D:435:PRO:HB2	1.79	1.11
1:C:203:GLY:HA3	1:C:330:VAL:HG22	1.20	1.10
1:C:330:VAL:HG12	1:C:331:TRP:HB3	1.32	1.08
1:C:203:GLY:HA2	1:C:330:VAL:HG21	1.33	1.08
1:C:203:GLY:CA	1:C:330:VAL:HG22	1.88	1.01
1:C:203:GLY:CA	1:C:330:VAL:HG21	1.92	0.98
1:D:479:ASN:HB2	5:D:1572:BBK:H4	1.44	0.98
1:D:271:LYS:HG2	1:D:301:ILE:HD11	1.46	0.96
1:C:330:VAL:HG11	6:C:1569:HWU:C5	1.99	0.92
1:C:145:HIS:CD2	1:C:201:ARG:HH21	1.91	0.89
1:A:479:ASN:HB2	5:A:1581:BBK:H4	1.54	0.88
1:E:479:ASN:HD22	5:E:1584:BBK:H3	1.39	0.86
1:A:291:ARG:CZ	1:D:435:PRO:CB	2.54	0.85
1:E:479:ASN:HB2	5:E:1584:BBK:H4	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASN:HD22	5:A:1581:BBK:H3	1.45	0.81
1:C:203:GLY:HA2	1:C:330:VAL:CG2	2.03	0.80
1:F:134:ASP:O	1:F:134:ASP:OD1	2.00	0.80
1:B:479:ASN:HB2	5:B:1580:BBK:H4	1.65	0.80
1:F:438:ARG:HG2	1:F:481:GLU:OE2	1.82	0.79
1:F:524:GLN:HG2	1:F:528:ASN:HA	1.63	0.78
1:F:474:HIS:HD2	1:F:476:ALA:H	1.30	0.78
1:C:114:MET:HA	7:C:2004:HOH:O	1.84	0.78
1:D:123:HIS:HD2	1:D:125:GLN:H	1.32	0.77
1:D:438:ARG:HG2	1:D:481:GLU:OE2	1.83	0.77
1:C:474:HIS:HD2	1:C:476:ALA:H	1.30	0.77
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.20	0.77
1:A:438:ARG:HG2	1:A:481:GLU:OE2	1.86	0.76
1:A:439:VAL:H	1:D:291:ARG:NH2	1.84	0.75
1:F:123:HIS:HD2	1:F:125:GLN:H	1.33	0.74
1:B:438:ARG:HG2	1:B:481:GLU:OE2	1.88	0.74
1:D:165:PRO:HA	4:D:1576:EDO:H22	1.69	0.74
1:D:479:ASN:HD22	5:D:1572:BBK:H3	1.52	0.74
1:C:123:HIS:HD2	1:C:125:GLN:H	1.36	0.74
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.22	0.73
6:B:1571:HWU:H1'	2:X:6:THR:OG1	1.88	0.73
1:E:123:HIS:HD2	1:E:125:GLN:H	1.33	0.72
1:D:516:ASP:OD1	1:D:516:ASP:N	2.22	0.72
1:A:123:HIS:HD2	1:A:125:GLN:H	1.36	0.72
1:B:123:HIS:HD2	1:B:125:GLN:H	1.37	0.72
1:A:291:ARG:NH1	1:D:435:PRO:HB2	2.05	0.71
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.25	0.71
6:C:1569:HWU:O3A	6:C:1569:HWU:H5'	1.91	0.70
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.25	0.70
1:D:277:ASN:ND2	1:D:279:VAL:HG12	2.06	0.70
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.26	0.70
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.25	0.70
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.57	0.69
1:E:438:ARG:HG2	1:E:481:GLU:OE2	1.93	0.69
1:C:277:ASN:ND2	1:C:279:VAL:HG12	2.08	0.69
4:B:1573:EDO:H12	7:B:2011:HOH:O	1.92	0.68
1:C:439:VAL:C	1:C:440:PRO:O	2.30	0.68
1:F:316:PHE:CE2	1:F:320:GLU:OE2	2.47	0.68
1:A:320:GLU:C	1:A:321:LEU:O	2.28	0.67
1:C:145:HIS:CE1	1:C:201:ARG:HE	2.12	0.67
1:C:439:VAL:O	1:C:440:PRO:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:THR:OG1	1:D:289:GLN:HG2	1.95	0.66
1:D:329:ASP:H	1:D:380:ASN:HD21	1.41	0.66
1:E:458:ASP:OD1	5:E:1584:BBK:O3	2.14	0.66
1:B:479:ASN:HD22	5:B:1580:BBK:H3	1.60	0.65
1:C:204:LEU:H	1:C:330:VAL:HG13	1.62	0.65
1:C:329:ASP:H	1:C:380:ASN:HD21	1.45	0.65
1:C:225:SER:O	1:C:226:HIS:CG	2.51	0.64
1:C:439:VAL:O	1:C:440:PRO:C	2.37	0.63
6:E:1585:HWU:H1'	2:Y:6:THR:HB	1.80	0.63
1:B:458:ASP:OD1	5:B:1580:BBK:O3	2.17	0.62
1:C:205:MET:HE3	1:C:328:MET:O	2.00	0.62
1:F:368:THR:HG22	1:F:370:PRO:HD3	1.82	0.62
6:C:1569:HWU:O3A	6:C:1569:HWU:O6'	2.18	0.62
1:A:263:TYR:H	4:A:1580:EDO:H21	1.65	0.62
1:A:194[B]:ARG:HG2	1:A:194[B]:ARG:HH11	1.65	0.62
1:F:329:ASP:H	1:F:380:ASN:HD21	1.48	0.62
1:B:316:PHE:CE2	1:B:320:GLU:OE2	2.53	0.62
1:A:368:THR:HG22	1:A:370:PRO:HD3	1.82	0.62
1:B:162:LYS:HE3	4:B:1573:EDO:O2	1.99	0.61
1:F:460:LEU:CD2	1:F:471:TYR:CE2	2.84	0.61
1:E:329:ASP:H	1:E:380:ASN:HD21	1.48	0.61
1:E:368:THR:HG22	1:E:370:PRO:HD3	1.83	0.60
1:B:329:ASP:H	1:B:380:ASN:HD21	1.48	0.60
1:D:160:LEU:HA	4:D:1576:EDO:H12	1.83	0.60
1:C:316:PHE:CE2	1:C:320:GLU:OE2	2.55	0.60
1:B:305:MET:HE1	1:B:336:LEU:CD2	2.32	0.60
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.49	0.60
1:D:305:MET:HE1	1:D:336:LEU:CD2	2.32	0.59
1:A:329:ASP:H	1:A:380:ASN:HD21	1.50	0.59
1:C:145:HIS:CD2	1:C:201:ARG:NH2	2.67	0.59
1:D:277:ASN:HD21	1:D:279:VAL:HG12	1.66	0.59
1:D:414:ARG:HD3	7:D:2082:HOH:O	2.01	0.59
1:D:316:PHE:CE2	1:D:320:GLU:OE2	2.56	0.58
1:E:278:LEU:O	4:E:1572:EDO:C1	2.51	0.58
1:C:176:ASP:OD2	1:C:203:GLY:N	2.34	0.58
7:C:2001:HOH:O	1:E:113:ARG:NH2	2.34	0.58
1:D:305:MET:HE1	1:D:336:LEU:HD23	1.85	0.58
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.52	0.58
1:A:474:HIS:HB2	5:D:1572:BBK:H8A	1.86	0.57
1:A:560:SER:HB3	4:A:1579:EDO:H12	1.86	0.57
1:C:277:ASN:HD21	1:C:279:VAL:HG12	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:LEU:HD22	1:F:471:TYR:CE2	2.39	0.57
6:B:1571:HWU:C1'	2:X:6:THR:OG1	2.52	0.57
1:C:205:MET:HE2	1:C:205:MET:H	1.68	0.57
1:B:305:MET:HE1	1:B:336:LEU:HD23	1.86	0.57
1:C:77:ARG:CG	1:C:80:ASP:OD2	2.53	0.57
1:C:517:ASP:O	1:C:521:LYS:HE2	2.04	0.56
1:E:479:ASN:HD22	5:E:1584:BBK:C3	2.14	0.56
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.54	0.56
1:A:305:MET:HE1	1:A:336:LEU:CD2	2.36	0.56
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.54	0.56
1:E:333:GLY:N	4:E:1572:EDO:H21	2.21	0.56
1:E:438:ARG:CG	1:E:481:GLU:OE2	2.54	0.56
1:C:305:MET:HE1	1:C:336:LEU:CD2	2.36	0.55
1:C:305:MET:HE1	1:C:336:LEU:HD23	1.88	0.55
1:D:271:LYS:CG	1:D:301:ILE:HD11	2.29	0.55
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.54	0.55
6:E:1585:HWU:O1B	2:Y:5:SER:N	2.38	0.55
1:E:333:GLY:H	4:E:1572:EDO:H21	1.72	0.55
5:B:1580:BBK:H8A	1:E:474:HIS:HB2	1.89	0.54
1:A:305:MET:HE1	1:A:336:LEU:HD23	1.90	0.54
1:E:479:ASN:ND2	5:E:1584:BBK:H3	2.14	0.54
1:E:414:ARG:HD3	7:E:2102:HOH:O	2.05	0.54
6:C:1569:HWU:H6'	6:C:1569:HWU:PA	2.30	0.54
1:C:471:TYR:CD1	1:F:472:GLU:OE1	2.60	0.54
1:E:492:HIS:HA	4:E:1582:EDO:H11	1.90	0.53
1:C:331:TRP:HE1	1:C:365:HIS:CE1	2.26	0.53
1:C:471:TYR:OH	1:F:473:CYS:O	2.26	0.53
1:B:516:ASP:OD1	1:C:117:ALA:HB3	2.09	0.53
1:B:492:HIS:HA	4:B:1577:EDO:H21	1.91	0.52
1:A:479:ASN:ND2	5:A:1581:BBK:H3	2.21	0.52
1:B:462:HIS:HD2	1:B:467:VAL:O	1.92	0.52
1:E:124:ASP:HB3	1:E:128:ARG:NH2	2.25	0.52
1:D:479:ASN:ND2	5:D:1572:BBK:H3	2.24	0.52
1:C:270:LEU:HD21	1:F:463:PHE:CE1	2.45	0.52
1:A:364:GLN:HE21	4:A:1572:EDO:C1	2.22	0.52
1:D:163:SER:O	4:D:1576:EDO:O1	2.28	0.52
1:C:77:ARG:H	1:C:77:ARG:CD	2.22	0.52
1:E:462:HIS:HD2	1:E:467:VAL:O	1.93	0.52
1:C:329:ASP:O	1:C:330:VAL:C	2.46	0.51
1:E:364:GLN:HE21	4:E:1573:EDO:H22	1.75	0.51
1:F:127:GLN:C	1:F:128:ARG:HD3	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:THR:OG1	1:D:289:GLN:CG	2.59	0.51
6:C:1569:HWU:PA	6:C:1569:HWU:O6'	2.68	0.51
1:E:333:GLY:HA2	4:E:1572:EDO:C2	2.40	0.51
1:C:471:TYR:CE2	1:F:472:GLU:HB3	2.46	0.51
1:D:414:ARG:CD	7:D:2082:HOH:O	2.57	0.50
1:A:291:ARG:NH2	1:D:435:PRO:CB	2.73	0.50
1:E:500:VAL:O	4:E:1580:EDO:H22	2.12	0.50
1:A:493:MET:HB3	1:D:269:ASP:OD2	2.12	0.49
1:B:158:SER:HB3	4:B:1573:EDO:H11	1.94	0.49
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.59	0.49
1:E:333:GLY:H	4:E:1572:EDO:C2	2.25	0.49
1:C:515:GLU:O	1:C:521:LYS:NZ	2.36	0.49
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.47	0.49
1:B:491:LYS:HE2	1:B:513:CYS:SG	2.52	0.49
1:A:491:LYS:HE2	1:A:513:CYS:SG	2.52	0.49
1:C:462:HIS:HD2	1:C:467:VAL:O	1.95	0.48
1:E:293:ARG:HD2	4:E:1570:EDO:H22	1.95	0.48
1:C:412:GLN:HB3	7:C:2013:HOH:O	2.13	0.48
1:A:305:MET:HE3	1:A:305:MET:HB2	1.61	0.48
1:D:305:MET:CE	1:D:336:LEU:HD23	2.44	0.48
1:A:305:MET:CE	1:A:336:LEU:HD23	2.43	0.48
1:C:305:MET:CE	1:C:336:LEU:HD23	2.43	0.48
1:D:235:GLU:N	1:D:236:PRO:CD	2.77	0.48
1:A:364:GLN:HE21	4:A:1572:EDO:H12	1.79	0.48
1:C:412:GLN:CB	7:C:2013:HOH:O	2.62	0.48
1:A:200:ARG:NH1	1:A:200:ARG:HG2	2.26	0.47
1:A:462:HIS:HD2	1:A:467:VAL:O	1.96	0.47
1:F:491:LYS:HE2	1:F:513:CYS:SG	2.54	0.47
1:F:538:LEU:HB3	1:F:552:VAL:HG22	1.96	0.47
1:A:343:TRP:CD1	1:A:349:LEU:HD22	2.49	0.47
1:E:239:GLU:OE2	7:E:2030:HOH:O	2.20	0.47
1:C:491:LYS:HE2	1:C:513:CYS:SG	2.54	0.47
1:B:343:TRP:CD1	1:B:349:LEU:HD22	2.49	0.47
1:C:204:LEU:HD12	1:C:205:MET:N	2.29	0.47
1:F:204:LEU:HD12	1:F:205:MET:N	2.29	0.47
1:C:331:TRP:CZ2	1:C:365:HIS:CG	3.02	0.47
1:E:305:MET:HB2	1:E:305:MET:HE3	1.60	0.47
1:E:278:LEU:O	4:E:1572:EDO:H12	2.14	0.47
1:B:305:MET:HB2	1:B:305:MET:HE3	1.69	0.47
1:C:77:ARG:NE	1:C:80:ASP:OD2	2.46	0.47
1:E:305:MET:CE	1:E:336:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:HA	1:A:291:ARG:NH1	2.30	0.47
1:F:343:TRP:CD1	1:F:349:LEU:HD22	2.50	0.47
1:A:277:ASN:O	4:A:1575:EDO:O1	2.20	0.47
1:E:333:GLY:HA2	4:E:1572:EDO:H22	1.97	0.47
1:B:178:SER:O	1:B:197:ARG:NH2	2.42	0.47
1:E:491:LYS:HE2	1:E:513:CYS:SG	2.54	0.47
1:E:305:MET:HE1	1:E:336:LEU:CD2	2.45	0.46
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.96	0.46
1:D:165:PRO:CA	4:D:1576:EDO:H22	2.44	0.46
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.98	0.46
1:C:155:THR:HG1	1:C:226:HIS:N	2.14	0.46
1:D:491:LYS:HE2	1:D:513:CYS:SG	2.55	0.46
1:A:291:ARG:NH2	1:D:435:PRO:HB2	2.27	0.46
1:A:439:VAL:H	1:D:291:ARG:HH21	1.59	0.46
1:F:178:SER:O	1:F:197:ARG:NH2	2.43	0.46
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.51	0.46
1:F:309:GLY:C	1:F:310:LEU:HD23	2.36	0.46
1:E:178:SER:O	1:E:197:ARG:NH2	2.42	0.46
1:C:205:MET:CE	1:C:328:MET:O	2.64	0.45
1:A:319:GLU:O	1:A:321:LEU:O	2.34	0.45
1:A:309:GLY:C	1:A:310:LEU:HD23	2.36	0.45
1:A:191:GLU:O	1:A:191:GLU:HG3	2.16	0.45
1:D:274:PHE:CD2	1:D:305:MET:HE1	2.51	0.45
1:C:305:MET:HE3	1:C:305:MET:HB2	1.64	0.45
1:E:493:MET:H	4:E:1582:EDO:H22	1.80	0.45
1:E:414:ARG:CD	7:E:2102:HOH:O	2.63	0.45
1:C:178:SER:O	1:C:197:ARG:NH2	2.40	0.45
1:C:204:LEU:HG	1:C:330:VAL:HG13	1.97	0.45
1:D:465:ASP:OD1	4:D:1573:EDO:H11	2.17	0.44
1:E:309:GLY:C	1:E:310:LEU:HD23	2.38	0.44
1:F:235:GLU:N	1:F:236:PRO:CD	2.80	0.44
1:C:189:LYS:NZ	7:C:2008:HOH:O	2.49	0.44
1:E:191:GLU:O	1:E:191:GLU:HG3	2.17	0.44
1:C:303:THR:HA	1:C:304:PRO:HD3	1.96	0.44
1:D:331:TRP:NE1	6:D:1571:HWU:H5'	2.33	0.44
1:D:285:MET:O	1:D:290:ARG:NH1	2.51	0.44
1:A:103:LYS:HD2	4:A:1572:EDO:H12	1.98	0.44
1:A:204:LEU:HD12	1:A:205:MET:N	2.32	0.44
1:C:106:GLN:HB2	7:C:2003:HOH:O	2.17	0.44
1:B:518:SER:HB3	1:C:161:LYS:NZ	2.32	0.44
1:A:178:SER:O	1:A:197:ARG:NH2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:N	4:A:1580:EDO:H21	2.31	0.44
1:B:305:MET:CE	1:B:336:LEU:HD23	2.47	0.44
1:B:235:GLU:N	1:B:236:PRO:CD	2.81	0.44
1:A:252:ILE:HG23	4:A:1578:EDO:H11	2.00	0.44
1:E:335:ASN:HD21	4:E:1572:EDO:C2	2.31	0.44
1:D:132:ARG:HB2	1:D:134:ASP:OD1	2.18	0.43
1:D:538:LEU:HB3	1:D:552:VAL:HG22	1.98	0.43
1:D:305:MET:HE3	1:D:305:MET:HB2	1.62	0.43
1:B:538:LEU:HB3	1:B:552:VAL:HG22	2.00	0.43
1:C:77:ARG:H	1:C:77:ARG:HD3	1.81	0.43
1:C:176:ASP:OD1	1:C:202:GLU:N	2.38	0.43
1:C:200:ARG:O	1:C:202:GLU:HG2	2.19	0.43
1:C:205:MET:HE3	1:C:205:MET:HB2	1.86	0.43
1:E:335:ASN:N	1:E:335:ASN:HD22	2.16	0.43
1:D:153:LEU:O	1:D:157:VAL:HG13	2.19	0.43
1:C:143:THR:HG1	6:C:1569:HWU:H1B	1.83	0.43
1:C:143:THR:OG1	6:C:1569:HWU:H1B	2.18	0.43
6:C:1569:HWU:O3A	6:C:1569:HWU:C5'	2.62	0.43
1:C:191:GLU:O	1:C:191:GLU:HG3	2.19	0.43
1:E:235:GLU:N	1:E:236:PRO:CD	2.81	0.43
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.53	0.43
1:B:375:THR:HG23	7:B:2079:HOH:O	2.18	0.43
1:C:205:MET:CE	1:C:205:MET:H	2.32	0.42
1:F:191:GLU:O	1:F:191:GLU:HG3	2.18	0.42
1:D:178:SER:O	1:D:197:ARG:NH2	2.40	0.42
1:C:285:MET:O	1:C:290:ARG:NH1	2.52	0.42
1:A:291:ARG:NE	1:D:435:PRO:CB	2.82	0.42
4:B:1573:EDO:C1	7:B:2011:HOH:O	2.59	0.42
6:D:1571:HWU:C5B	6:D:1571:HWU:H6	2.49	0.42
6:D:1571:HWU:H5B1	6:D:1571:HWU:H6	1.99	0.42
6:D:1571:HWU:H5B2	6:D:1571:HWU:HA	1.84	0.42
1:D:204:LEU:HD13	1:D:331:TRP:HA	2.02	0.42
1:D:191:GLU:HG3	1:D:191:GLU:O	2.20	0.42
1:E:538:LEU:HB3	1:E:552:VAL:HG22	2.01	0.42
1:C:309:GLY:C	1:C:310:LEU:HD23	2.39	0.42
1:A:364:GLN:NE2	4:A:1572:EDO:H12	2.34	0.42
6:F:1571:HWU:H5B2	6:F:1571:HWU:H6	2.02	0.42
1:F:309:GLY:CA	6:F:1571:HWU:O3'	2.67	0.42
1:E:153:LEU:O	1:E:157:VAL:HG13	2.19	0.42
1:E:377:PHE:CE2	4:E:1579:EDO:H21	2.54	0.42
1:E:285:MET:O	1:E:290:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLY:C	1:B:310:LEU:HD23	2.39	0.42
1:C:331:TRP:NE1	1:C:365:HIS:CE1	2.88	0.42
1:A:439:VAL:HG13	1:D:291:ARG:NH2	2.35	0.42
1:C:330:VAL:HG11	6:C:1569:HWU:H5	1.93	0.42
1:E:305:MET:CE	1:E:336:LEU:CD2	2.98	0.42
1:D:86:TYR:CE2	1:D:149:ARG:HB3	2.55	0.42
1:A:153:LEU:O	1:A:157:VAL:HG13	2.20	0.42
1:C:224:ASP:OD2	6:C:1569:HWU:O2B	2.37	0.42
1:E:305:MET:HE1	1:E:336:LEU:HD23	2.00	0.42
1:D:502:ARG:HD2	7:D:2111:HOH:O	2.18	0.42
1:A:285:MET:O	1:A:290:ARG:NH1	2.53	0.42
1:D:450:LEU:HD13	1:D:563:TRP:CE3	2.55	0.42
1:F:285:MET:O	1:F:290:ARG:NH1	2.53	0.42
2:X:7:CYS:HA	2:X:8:PRO:HD3	1.89	0.42
1:C:291:ARG:NE	1:F:435:PRO:HB2	2.34	0.41
1:C:330:VAL:HG11	6:C:1569:HWU:C4	2.48	0.41
1:A:305:MET:CE	1:A:336:LEU:CD2	2.97	0.41
1:B:285:MET:O	1:B:290:ARG:NH1	2.53	0.41
1:B:130:GLN:HB3	1:B:130:GLN:HE21	1.67	0.41
1:F:153:LEU:O	1:F:157:VAL:HG13	2.19	0.41
1:A:439:VAL:H	1:D:291:ARG:HH22	1.64	0.41
1:C:225:SER:O	1:C:226:HIS:ND1	2.53	0.41
1:C:305:MET:CE	1:C:336:LEU:CD2	2.98	0.41
1:F:514:ARG:C	1:F:516:ASP:H	2.24	0.41
1:C:204:LEU:N	1:C:330:VAL:HG13	2.31	0.41
1:B:450:LEU:HD13	1:B:563:TRP:CE3	2.55	0.41
1:A:457:LEU:HD13	1:A:482:TRP:CZ2	2.56	0.41
1:D:309:GLY:C	1:D:310:LEU:HD23	2.41	0.41
1:F:460:LEU:HD23	1:F:471:TYR:CE2	2.56	0.41
1:E:377:PHE:CE2	4:E:1579:EDO:C2	3.04	0.41
1:B:511:GLN:NE2	4:B:1572:EDO:H21	2.36	0.41
1:C:515:GLU:O	1:C:517:ASP:N	2.54	0.41
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.56	0.41
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.17	0.40
1:D:83:GLN:HG2	1:D:84:GLU:N	2.35	0.40
1:C:271:LYS:HB2	1:C:271:LYS:HE3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/571 (86%)	479 (97%)	14 (3%)	1 (0%)	52	59
1	B	493/571 (86%)	476 (97%)	16 (3%)	1 (0%)	52	59
1	C	470/571 (82%)	451 (96%)	16 (3%)	3 (1%)	30	29
1	D	493/571 (86%)	478 (97%)	14 (3%)	1 (0%)	52	59
1	E	493/571 (86%)	479 (97%)	13 (3%)	1 (0%)	52	59
1	F	487/571 (85%)	473 (97%)	13 (3%)	1 (0%)	52	59
2	X	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	Y	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	2938/3438 (86%)	2842 (97%)	88 (3%)	8 (0%)	46	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	C	440	PRO
1	B	330	VAL
1	C	332	GLY
1	C	516	ASP
1	D	330	VAL
1	F	330	VAL
1	E	330	VAL

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	429/485 (88%)	388 (90%)	41 (10%)	10 9
1	B	428/485 (88%)	390 (91%)	38 (9%)	12 11
1	C	414/485 (85%)	371 (90%)	43 (10%)	9 8
1	D	428/485 (88%)	385 (90%)	43 (10%)	9 8
1	E	428/485 (88%)	389 (91%)	39 (9%)	12 11
1	F	424/485 (87%)	382 (90%)	42 (10%)	10 9
2	X	4/4 (100%)	3 (75%)	1 (25%)	1 0
2	Y	4/4 (100%)	2 (50%)	2 (50%)	0 0
All	All	2559/2918 (88%)	2310 (90%)	249 (10%)	10 9

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	76	VAL
1	A	77	ARG
1	A	101	ARG
1	A	112	LEU
1	A	116	ARG
1	A	124	ASP
1	A	133	VAL
1	A	173	LEU
1	A	195	VAL
1	A	196	LEU
1	A	200	ARG
1	A	204	LEU
1	A	241	VAL
1	A	277	ASN
1	A	288	GLU
1	A	296	ASN
1	A	302	LYS
1	A	310	LEU
1	A	330	VAL
1	A	335	ASN
1	A	336	LEU
1	A	349	LEU
1	A	410	ASN
1	A	414	ARG
1	A	419	LYS
1	A	421	LEU

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Mol	Chain	Res	Type
1	A	438	ARG
1	A	439	VAL
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	471	TYR
1	A	484	LEU
1	A	502	ARG
1	A	510	LEU
1	A	515	GLU
1	A	546	LYS
1	A	552	VAL
1	A	554	VAL
1	A	567	LEU
1	B	75	LYS
1	B	76	VAL
1	B	101	ARG
1	B	112	LEU
1	B	116	ARG
1	B	124	ASP
1	B	130	GLN
1	B	133	VAL
1	B	143	THR
1	B	173	LEU
1	B	195	VAL
1	B	196	LEU
1	B	204	LEU
1	B	277	ASN
1	B	288	GLU
1	B	296	ASN
1	B	302	LYS
1	B	310	LEU
1	B	335	ASN
1	B	336	LEU
1	B	349	LEU
1	B	375	THR
1	B	410	ASN
1	B	414	ARG
1	B	419	LYS
1	B	421	LEU
1	B	438	ARG
1	B	439	VAL

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Mol	Chain	Res	Type
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	471	TYR
1	B	484	LEU
1	B	502	ARG
1	B	510	LEU
1	B	552	VAL
1	B	554	VAL
1	B	567	LEU
1	C	75	LYS
1	C	76	VAL
1	C	77	ARG
1	C	101	ARG
1	C	112	LEU
1	C	113	ARG
1	C	116	ARG
1	C	124	ASP
1	C	133	VAL
1	C	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	201	ARG
1	C	204	LEU
1	C	205	MET
1	C	277	ASN
1	C	288	GLU
1	C	294	GLN
1	C	296	ASN
1	C	302	LYS
1	C	310	LEU
1	C	330	VAL
1	C	335	ASN
1	C	336	LEU
1	C	349	LEU
1	C	410	ASN
1	C	419	LYS
1	C	421	LEU
1	C	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	457	LEU

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Mol	Chain	Res	Type
1	C	468	VAL
1	C	471	TYR
1	C	484	LEU
1	C	500	VAL
1	C	502	ARG
1	C	510	LEU
1	C	515	GLU
1	C	516	ASP
1	C	546	LYS
1	C	552	VAL
1	C	554	VAL
1	D	75	LYS
1	D	76	VAL
1	D	101	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	173	LEU
1	D	195	VAL
1	D	196	LEU
1	D	204	LEU
1	D	277	ASN
1	D	284	TYR
1	D	288	GLU
1	D	289	GLN
1	D	291	ARG
1	D	294	GLN
1	D	296	ASN
1	D	301	ILE
1	D	302	LYS
1	D	310	LEU
1	D	335	ASN
1	D	336	LEU
1	D	349	LEU
1	D	375	THR
1	D	410	ASN
1	D	419	LYS
1	D	421	LEU
1	D	438	ARG
1	D	439	VAL
1	D	450	LEU

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Mol	Chain	Res	Type
1	D	457	LEU
1	D	468	VAL
1	D	471	TYR
1	D	484	LEU
1	D	502	ARG
1	D	510	LEU
1	D	515	GLU
1	D	516	ASP
1	D	546	LYS
1	D	552	VAL
1	D	554	VAL
1	D	568	ASN
1	E	75	LYS
1	E	76	VAL
1	E	77	ARG
1	E	101	ARG
1	E	112	LEU
1	E	116	ARG
1	E	124	ASP
1	E	133	VAL
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	204	LEU
1	E	277	ASN
1	E	288	GLU
1	E	294	GLN
1	E	296	ASN
1	E	302	LYS
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	375	THR
1	E	410	ASN
1	E	419	LYS
1	E	421	LEU
1	E	438	ARG
1	E	439	VAL
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL

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Mol	Chain	Res	Type
1	E	471	TYR
1	E	484	LEU
1	E	502	ARG
1	E	510	LEU
1	E	515	GLU
1	E	546	LYS
1	E	552	VAL
1	E	554	VAL
1	E	567	LEU
1	F	75	LYS
1	F	76	VAL
1	F	101	ARG
1	F	112	LEU
1	F	116	ARG
1	F	124	ASP
1	F	128	ARG
1	F	134	ASP
1	F	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	204	LEU
1	F	277	ASN
1	F	288	GLU
1	F	294	GLN
1	F	296	ASN
1	F	302	LYS
1	F	310	LEU
1	F	335	ASN
1	F	336	LEU
1	F	349	LEU
1	F	375	THR
1	F	410	ASN
1	F	414	ARG
1	F	419	LYS
1	F	421	LEU
1	F	438	ARG
1	F	439	VAL
1	F	442	HIS
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	471	TYR

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Mol	Chain	Res	Type
1	F	484	LEU
1	F	500	VAL
1	F	502	ARG
1	F	510	LEU
1	F	515	GLU
1	F	516	ASP
1	F	546	LYS
1	F	552	VAL
1	F	554	VAL
2	X	5	SER
2	Y	6	THR
2	Y	7	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	123	HIS
1	A	127	GLN
1	A	198	ASN
1	A	277	ASN
1	A	296	ASN
1	A	335	ASN
1	A	344	GLN
1	A	364	GLN
1	A	365	HIS
1	A	380	ASN
1	A	410	ASN
1	A	432	ASN
1	A	452	GLN
1	A	462	HIS
1	A	479	ASN
1	A	537	ASN
1	B	106	GLN
1	B	123	HIS
1	B	127	GLN
1	B	130	GLN
1	B	198	ASN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN

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Mol	Chain	Res	Type
1	B	365	HIS
1	B	380	ASN
1	B	410	ASN
1	B	451	GLN
1	B	452	GLN
1	B	462	HIS
1	B	479	ASN
1	B	537	ASN
1	C	106	GLN
1	C	123	HIS
1	C	127	GLN
1	C	198	ASN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	365	HIS
1	C	410	ASN
1	C	451	GLN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	537	ASN
1	D	106	GLN
1	D	123	HIS
1	D	127	GLN
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	365	HIS
1	D	380	ASN
1	D	410	ASN
1	D	432	ASN
1	D	451	GLN
1	D	452	GLN
1	D	479	ASN
1	E	102	ASN
1	E	106	GLN
1	E	123	HIS
1	E	127	GLN

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Mol	Chain	Res	Type
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	364	GLN
1	E	365	HIS
1	E	380	ASN
1	E	410	ASN
1	E	451	GLN
1	E	452	GLN
1	E	462	HIS
1	E	479	ASN
1	E	537	ASN
1	F	106	GLN
1	F	123	HIS
1	F	127	GLN
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	365	HIS
1	F	380	ASN
1	F	410	ASN
1	F	432	ASN
1	F	451	GLN
1	F	452	GLN
1	F	474	HIS
1	F	537	ASN
1	F	562	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)

Of 53 ligands modelled in this entry, 6 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	A	1571	-	3,3,3	0.86	0	2,2,2	0.27	0
4	EDO	A	1572	-	3,3,3	0.51	0	2,2,2	0.60	0
4	EDO	A	1573	-	3,3,3	0.81	0	2,2,2	0.06	0
4	EDO	A	1574	-	3,3,3	0.54	0	2,2,2	0.15	0
4	EDO	A	1575	-	3,3,3	0.37	0	2,2,2	0.72	0
4	EDO	A	1576	-	3,3,3	0.31	0	2,2,2	0.82	0
4	EDO	A	1577	-	3,3,3	0.56	0	2,2,2	0.18	0
4	EDO	A	1578	-	3,3,3	0.70	0	2,2,2	0.63	0
4	EDO	A	1579	-	3,3,3	0.69	0	2,2,2	0.45	0
4	EDO	A	1580	-	3,3,3	0.95	0	2,2,2	1.16	0
5	BBK	A	1581	-	12,15,15	7.47	1 (8%)	15,21,21	2.08	5 (33%)
6	HWU	A	1582	3	30,41,41	3.90	4 (13%)	41,62,62	1.66	10 (24%)
6	HWU	B	1571	3	30,41,41	3.94	7 (23%)	41,62,62	2.15	13 (31%)
4	EDO	B	1572	-	3,3,3	0.52	0	2,2,2	0.59	0
4	EDO	B	1573	-	3,3,3	0.28	0	2,2,2	0.34	0
4	EDO	B	1574	-	3,3,3	0.61	0	2,2,2	0.39	0
4	EDO	B	1575	-	3,3,3	0.45	0	2,2,2	0.42	0
4	EDO	B	1576	-	3,3,3	0.64	0	2,2,2	0.17	0
4	EDO	B	1577	-	3,3,3	0.28	0	2,2,2	1.18	0
4	EDO	B	1578	-	3,3,3	0.55	0	2,2,2	0.44	0
4	EDO	B	1579	-	3,3,3	0.70	0	2,2,2	0.07	0
5	BBK	B	1580	-	12,15,15	7.53	1 (8%)	15,21,21	1.85	3 (20%)
6	HWU	C	1569	3	30,41,41	5.05	3 (10%)	41,62,62	2.37	15 (36%)
6	HWU	D	1571	3	30,41,41	4.49	5 (16%)	41,62,62	2.44	14 (34%)
5	BBK	D	1572	-	12,15,15	7.87	1 (8%)	15,21,21	3.21	5 (33%)
4	EDO	D	1573	-	3,3,3	0.50	0	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	D	1574	-	3,3,3	0.80	0	2,2,2	0.49	0
4	EDO	D	1575	-	3,3,3	0.90	0	2,2,2	0.34	0
4	EDO	D	1576	-	3,3,3	0.59	0	2,2,2	0.57	0
4	EDO	D	1577	-	3,3,3	0.46	0	2,2,2	0.74	0
4	EDO	E	1570	-	3,3,3	0.75	0	2,2,2	0.39	0
4	EDO	E	1571	-	3,3,3	0.68	0	2,2,2	0.23	0
4	EDO	E	1572	-	3,3,3	0.41	0	2,2,2	0.44	0
4	EDO	E	1573	-	3,3,3	0.31	0	2,2,2	1.02	0
4	EDO	E	1574	-	3,3,3	0.37	0	2,2,2	0.89	0
4	EDO	E	1575	-	3,3,3	0.47	0	2,2,2	0.40	0
4	EDO	E	1576	-	3,3,3	0.54	0	2,2,2	0.59	0
4	EDO	E	1577	-	3,3,3	0.36	0	2,2,2	0.82	0
4	EDO	E	1578	-	3,3,3	0.41	0	2,2,2	0.74	0
4	EDO	E	1579	-	3,3,3	0.47	0	2,2,2	0.61	0
4	EDO	E	1580	-	3,3,3	0.64	0	2,2,2	0.29	0
4	EDO	E	1581	-	3,3,3	0.36	0	2,2,2	0.93	0
4	EDO	E	1582	-	3,3,3	0.37	0	2,2,2	0.36	0
4	EDO	E	1583	-	3,3,3	0.59	0	2,2,2	0.17	0
5	BBK	E	1584	-	12,15,15	7.74	1 (8%)	15,21,21	2.05	5 (33%)
6	HWU	E	1585	3	30,41,41	4.02	4 (13%)	41,62,62	1.57	8 (19%)
6	HWU	F	1571	3	30,41,41	3.86	5 (16%)	41,62,62	1.60	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1571	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1579	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1580	-	-	0/1/1/1	0/0/0/0
5	BBK	A	1581	-	-	2/5/26/26	0/1/1/1
6	HWU	A	1582	3	-	0/20/63/63	0/3/3/3
6	HWU	B	1571	3	-	0/20/63/63	0/3/3/3
4	EDO	B	1572	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1579	-	-	0/1/1/1	0/0/0/0
5	BBK	B	1580	-	-	0/5/26/26	0/1/1/1
6	HWU	C	1569	3	-	0/20/63/63	0/3/3/3
6	HWU	D	1571	3	-	0/20/63/63	0/3/3/3
5	BBK	D	1572	-	-	0/5/26/26	0/1/1/1
4	EDO	D	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1570	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1571	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1579	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1580	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1581	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1582	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1583	-	-	0/1/1/1	0/0/0/0
5	BBK	E	1584	-	-	0/5/26/26	0/1/1/1
6	HWU	E	1585	3	-	0/20/63/63	0/3/3/3
6	HWU	F	1571	3	-	0/20/63/63	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1569	HWU	C5'-S5'	-27.24	1.41	1.82
5	D	1572	BBK	C5-S5	-27.03	1.42	1.82
5	E	1584	BBK	C5-S5	-26.64	1.42	1.82
5	B	1580	BBK	C5-S5	-25.96	1.43	1.82
5	A	1581	BBK	C5-S5	-25.79	1.43	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1571	HWU	C5'-S5'	-23.15	1.47	1.82
6	E	1585	HWU	C5'-S5'	-20.86	1.51	1.82
6	A	1582	HWU	C5'-S5'	-20.51	1.51	1.82
6	F	1571	HWU	C5'-S5'	-20.20	1.52	1.82
6	B	1571	HWU	C5'-S5'	-20.16	1.52	1.82
6	B	1571	HWU	C6-N1	-3.45	1.30	1.35
6	B	1571	HWU	O5B-C5B	-2.56	1.34	1.44
6	B	1571	HWU	PB-O2B	-2.55	1.44	1.54
6	D	1571	HWU	O5B-C5B	-2.49	1.34	1.44
6	A	1582	HWU	PB-O1B	-2.20	1.43	1.51
6	C	1569	HWU	PB-O2B	-2.15	1.45	1.54
6	E	1585	HWU	PB-O2B	-2.13	1.45	1.54
6	F	1571	HWU	O5B-C5B	-2.08	1.36	1.44
6	A	1582	HWU	C4-N3	2.08	1.37	1.33
6	C	1569	HWU	O4B-C1B	2.14	1.43	1.41
6	B	1571	HWU	PB-O1'	2.32	1.66	1.60
6	F	1571	HWU	C4-N3	2.37	1.37	1.33
6	E	1585	HWU	C4'-C5'	2.42	1.55	1.53
6	F	1571	HWU	C4'-C5'	2.51	1.55	1.53
6	A	1582	HWU	C6'-C5'	2.55	1.54	1.52
6	B	1571	HWU	C4'-C5'	2.65	1.55	1.53
6	D	1571	HWU	O4B-C1B	2.65	1.44	1.41
6	B	1571	HWU	O4B-C1B	2.81	1.44	1.41
6	F	1571	HWU	O4B-C1B	3.02	1.45	1.41
6	D	1571	HWU	C6'-C5'	3.53	1.55	1.52
6	E	1585	HWU	O4B-C1B	4.50	1.46	1.41
6	D	1571	HWU	C4'-C5'	4.57	1.57	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1572	BBK	C1-C2-N2	-8.97	93.88	111.48
5	D	1572	BBK	O1-C1-C2	-7.00	93.37	109.23
6	C	1569	HWU	PB-O3A-PA	-5.38	117.62	132.73
6	D	1571	HWU	O3A-PA-O5B	-5.23	89.06	102.94
6	D	1571	HWU	O1'-PB-O1B	-4.33	92.43	109.46
5	E	1584	BBK	C1-C2-C3	-3.89	103.98	110.07
6	C	1569	HWU	O6'-C6'-C5'	-3.84	101.31	110.63
5	B	1580	BBK	C1-C2-C3	-3.80	104.13	110.07
5	E	1584	BBK	C3-C2-N2	-3.64	103.13	110.66
6	C	1569	HWU	C4B-O4B-C1B	-3.63	105.73	109.72
6	B	1571	HWU	O3A-PA-O5B	-3.48	93.71	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1571	HWU	O4B-C4B-C5B	-3.47	96.92	109.32
6	B	1571	HWU	O2A-PA-O5B	-3.33	91.68	108.46
6	C	1569	HWU	C1'-C2'-N2'	-3.29	104.42	111.17
6	A	1582	HWU	O3A-PB-O1'	-3.25	94.27	103.63
6	B	1571	HWU	C4'-C3'-C2'	-3.24	105.94	110.43
6	B	1571	HWU	O3A-PB-O1'	-3.21	94.40	103.63
6	F	1571	HWU	O3A-PA-O5B	-3.11	94.69	102.94
6	C	1569	HWU	C4'-C3'-C2'	-3.06	106.18	110.43
6	E	1585	HWU	O3A-PB-O1'	-3.06	94.83	103.63
6	F	1571	HWU	O4B-C4B-C5B	-2.99	98.62	109.32
6	D	1571	HWU	C6-N1-C2	-2.91	116.56	121.28
5	A	1581	BBK	C1-C2-C3	-2.72	105.81	110.07
6	D	1571	HWU	C5B-C4B-C3B	-2.70	104.51	115.21
6	D	1571	HWU	O4'-C4'-C3'	-2.64	104.39	110.34
6	A	1582	HWU	C2'-N2'-C7'	-2.63	116.36	123.10
6	B	1571	HWU	PB-O3A-PA	-2.57	125.51	132.73
6	B	1571	HWU	O4B-C4B-C5B	-2.57	100.14	109.32
6	B	1571	HWU	O4'-C4'-C3'	-2.55	104.59	110.34
6	A	1582	HWU	O1'-PB-O1B	-2.50	99.64	109.46
6	A	1582	HWU	C4'-C3'-C2'	-2.48	107.00	110.43
6	E	1585	HWU	O7'-C7'-C8'	-2.46	117.55	122.06
6	F	1571	HWU	C4'-C3'-C2'	-2.44	107.05	110.43
6	A	1582	HWU	O5B-PA-O1A	-2.29	100.71	109.62
5	E	1584	BBK	O6-C6-C5	-2.23	105.22	110.63
6	A	1582	HWU	C6'-C5'-C4'	-2.15	99.69	115.13
5	A	1581	BBK	C3-C2-N2	-2.13	106.25	110.66
6	E	1585	HWU	C4'-C3'-C2'	-2.13	107.47	110.43
6	A	1582	HWU	O7'-C7'-C8'	-2.11	118.19	122.06
6	C	1569	HWU	O7'-C7'-C8'	-2.09	118.22	122.06
6	D	1571	HWU	O3'-C3'-C4'	-2.09	105.64	110.34
6	D	1571	HWU	C5-C4-N3	-2.06	117.83	123.12
6	E	1585	HWU	C6-N1-C2	-2.02	118.01	121.28
6	D	1571	HWU	O3A-PB-O1'	-2.00	97.87	103.63
6	A	1582	HWU	O2B-PB-O3A	2.06	114.42	105.09
6	B	1571	HWU	O2B-PB-O3A	2.07	114.47	105.09
5	D	1572	BBK	O3-C3-C4	2.12	115.10	110.34
6	D	1571	HWU	O4'-C4'-C5'	2.12	113.67	108.83
6	C	1569	HWU	O5B-PA-O1A	2.18	118.06	109.62
5	D	1572	BBK	O4-C4-C5	2.32	114.12	108.83
6	D	1571	HWU	O5B-C5B-C4B	2.32	117.68	109.12
6	F	1571	HWU	O4B-C1B-N1	2.34	113.02	108.08
5	A	1581	BBK	O3-C3-C4	2.41	115.77	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1569	HWU	O4B-C4B-C3B	2.46	110.11	105.15
6	D	1571	HWU	PB-O3A-PA	2.54	139.86	132.73
6	E	1585	HWU	O7'-C7'-N2'	2.58	127.13	121.86
6	E	1585	HWU	O3'-C3'-C2'	2.60	114.96	109.66
6	B	1571	HWU	O7'-C7'-N2'	2.61	127.19	121.86
6	A	1582	HWU	O2B-PB-O1B	2.62	126.70	112.53
6	F	1571	HWU	O5B-PA-O1A	2.71	120.12	109.62
6	B	1571	HWU	C4-N3-C2	2.72	116.84	114.14
5	D	1572	BBK	C4-C3-C2	2.79	114.30	110.43
5	E	1584	BBK	C2-N2-C7	2.88	130.51	123.10
6	F	1571	HWU	O2B-PB-O3A	2.93	118.38	105.09
5	E	1584	BBK	O4-C4-C5	3.03	115.75	108.83
5	B	1580	BBK	C2-N2-C7	3.04	130.90	123.10
5	B	1580	BBK	O4-C4-C5	3.06	115.81	108.83
6	C	1569	HWU	O3B-C3B-C4B	3.11	120.38	111.05
6	E	1585	HWU	O1'-C1'-C2'	3.18	112.62	107.14
6	C	1569	HWU	C1'-C2'-C3'	3.23	118.65	109.74
6	C	1569	HWU	O2A-PA-O3A	3.29	120.04	105.09
6	C	1569	HWU	O4B-C1B-N1	3.40	115.24	108.08
6	C	1569	HWU	O3A-PB-O1'	3.54	113.82	103.63
6	B	1571	HWU	O1'-PB-O1B	3.86	124.64	109.46
6	E	1585	HWU	C4-N3-C2	3.98	118.08	114.14
6	D	1571	HWU	O3'-C3'-C2'	4.13	118.08	109.66
5	A	1581	BBK	C2-N2-C7	4.24	134.00	123.10
6	C	1569	HWU	O1'-C1'-C2'	4.47	114.84	107.14
5	A	1581	BBK	C1-C2-N2	4.50	120.31	111.48
6	F	1571	HWU	C4-N3-C2	4.61	118.71	114.14
6	B	1571	HWU	O1'-C1'-C2'	5.36	116.37	107.14
6	B	1571	HWU	O5B-PA-O1A	5.42	130.67	109.62
6	A	1582	HWU	C4-N3-C2	6.32	120.40	114.14
6	C	1569	HWU	C4-N3-C2	6.37	120.45	114.14
6	D	1571	HWU	C4-N3-C2	8.86	122.92	114.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1581	BBK	C8-C7-N2-C2
5	A	1581	BBK	O7-C7-N2-C2

There are no ring outliers.

25 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1572	EDO	4	0
4	A	1575	EDO	1	0
4	A	1578	EDO	1	0
4	A	1579	EDO	1	0
4	A	1580	EDO	2	0
5	A	1581	BBK	3	0
6	B	1571	HWU	2	0
4	B	1572	EDO	1	0
4	B	1573	EDO	4	0
4	B	1577	EDO	1	0
5	B	1580	BBK	4	0
6	C	1569	HWU	11	0
6	D	1571	HWU	4	0
5	D	1572	BBK	4	0
4	D	1573	EDO	1	0
4	D	1576	EDO	4	0
4	E	1570	EDO	1	0
4	E	1572	EDO	8	0
4	E	1573	EDO	1	0
4	E	1579	EDO	2	0
4	E	1580	EDO	1	0
4	E	1582	EDO	2	0
5	E	1584	BBK	5	0
6	E	1585	HWU	2	0
6	F	1571	HWU	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	495/571 (86%)	0.03	19 (3%) 44 43	26, 42, 70, 130	5 (1%)
1	B	495/571 (86%)	-0.05	15 (3%) 54 53	26, 40, 66, 106	5 (1%)
1	C	476/571 (83%)	2.07	198 (41%) 0 0	42, 92, 135, 168	5 (1%)
1	D	495/571 (86%)	0.01	19 (3%) 44 43	26, 41, 66, 142	5 (1%)
1	E	495/571 (86%)	-0.14	9 (1%) 71 70	23, 36, 58, 90	5 (1%)
1	F	491/571 (85%)	0.72	86 (17%) 2 2	34, 57, 112, 140	5 (1%)
2	X	6/6 (100%)	1.46	2 (33%) 0 0	40, 73, 84, 87	0
2	Y	6/6 (100%)	2.80	4 (66%) 0 0	42, 71, 77, 83	0
All	All	2959/3438 (86%)	0.44	352 (11%) 6 6	23, 45, 109, 168	30 (1%)

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	VAL	14.5
1	C	331	TRP	11.2
1	C	476	ALA	11.1
1	F	547	SER	10.6
1	F	556	GLY	9.2
1	C	423	CYS	8.9
1	C	400	VAL	8.9
1	F	557	PRO	8.9
1	C	475	ASN	8.4
1	C	516	ASP	7.9
1	C	442	HIS	7.9
1	C	497	LEU	7.8
1	F	503	ALA	7.4
1	C	471	TYR	7.3
1	C	443	GLN	7.2
1	C	284	TYR	6.9

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Mol	Chain	Res	Type	RSRZ
1	F	531	LEU	6.9
1	F	96	GLN	6.6
1	C	438	ARG	6.6
1	F	552	VAL	6.6
1	C	547	SER	6.4
1	C	101	ARG	6.3
1	C	531	LEU	6.3
1	C	410	ASN	6.3
1	C	417	LEU	6.2
1	C	514	ARG	6.2
1	C	405	ASN	6.1
1	A	291	ARG	6.0
1	C	403	ALA	6.0
1	F	95	GLY	6.0
1	F	559	LEU	6.0
1	C	99	TYR	5.9
1	C	546	LYS	5.9
1	D	284	TYR	5.8
1	D	287	PRO	5.8
1	C	440	PRO	5.8
1	C	534	VAL	5.8
1	C	406	VAL	5.8
1	F	540	LEU	5.7
1	C	98	PRO	5.7
1	C	408	TYR	5.7
1	C	513	CYS	5.7
1	F	537	ASN	5.6
1	C	117	ALA	5.6
1	C	177	TYR	5.6
1	F	475	ASN	5.5
1	F	516	ASP	5.4
1	F	94	SER	5.3
1	C	502	ARG	5.3
1	C	401	PRO	5.3
1	C	540	LEU	5.3
1	C	399	ALA	5.2
1	C	89	GLY	5.2
1	C	445	ILE	5.2
2	Y	7	CYS	5.2
1	F	504	PRO	5.1
1	F	525	ILE	5.1
1	C	456	CYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	516	ASP	5.1
1	C	457	LEU	5.0
1	F	501	ASP	5.0
1	F	555	CYS	5.0
1	C	421	LEU	5.0
1	F	127	GLN	5.0
1	D	291	ARG	5.0
1	C	453	GLY	4.9
1	C	364	GLN	4.9
1	C	413	SER	4.9
1	C	439	VAL	4.9
1	C	527	GLY	4.9
1	F	453	GLY	4.8
1	F	128	ARG	4.8
1	C	363	LYS	4.8
1	C	437	LEU	4.8
1	C	366	PRO	4.7
1	C	107	VAL	4.7
1	C	199	ASP	4.6
1	E	516	ASP	4.6
1	C	447	PHE	4.6
1	C	427	LYS	4.6
1	C	279	VAL	4.6
1	F	522	TRP	4.6
1	C	454	THR	4.6
1	C	493	MET	4.6
1	C	130	GLN	4.6
1	F	89	GLY	4.6
1	C	473	CYS	4.5
1	C	280	PHE	4.5
1	C	441	ASP	4.5
1	A	287	PRO	4.4
1	F	93	ARG	4.4
1	C	151	ALA	4.4
1	C	477	GLY	4.3
1	C	128	ARG	4.3
1	F	543	ARG	4.3
1	C	204	LEU	4.3
1	C	143	THR	4.3
1	C	419	LYS	4.2
1	F	442	HIS	4.2
1	C	522	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	554	VAL	4.2
1	C	548	GLY	4.2
1	C	383	ARG	4.2
1	C	495	LEU	4.2
2	X	6	THR	4.1
1	C	504	PRO	4.1
1	C	97	ASP	4.1
1	D	557	PRO	4.1
1	F	497	LEU	4.1
1	F	554	VAL	4.0
1	C	384	ALA	4.0
2	Y	6	THR	4.0
1	C	182	GLU	4.0
1	F	535	GLY	4.0
1	C	544	THR	4.0
1	F	515	GLU	4.0
1	C	100	ALA	3.9
1	C	533	HIS	3.9
1	C	463	PHE	3.9
1	F	287	PRO	3.9
1	A	295	GLY	3.9
1	C	144	PHE	3.9
1	C	566	THR	3.9
1	C	329	ASP	3.8
1	C	412	GLN	3.8
1	F	405	ASN	3.8
1	B	93	ARG	3.8
1	C	468	VAL	3.8
1	C	113	ARG	3.7
1	C	555	CYS	3.7
1	F	546	LYS	3.7
1	A	288	GLU	3.7
1	C	200	ARG	3.7
1	C	152	LEU	3.7
1	C	559	LEU	3.7
1	F	454	THR	3.7
1	C	396	TYR	3.7
1	C	411	ILE	3.6
1	F	544	THR	3.6
1	C	79	PRO	3.6
1	C	407	PRO	3.6
1	C	528	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	508	ILE	3.6
1	F	514	ARG	3.6
1	C	77	ARG	3.6
1	F	438	ARG	3.6
1	C	365	HIS	3.6
1	C	490	VAL	3.5
1	C	150	SER	3.5
1	C	340	PHE	3.5
1	F	527	GLY	3.5
1	C	508	ILE	3.5
1	C	536	SER	3.5
1	C	567	LEU	3.5
1	B	516	ASP	3.4
1	D	516	ASP	3.4
1	F	506	SER	3.4
1	C	474	HIS	3.4
1	F	476	ALA	3.4
1	B	371	GLY	3.4
1	F	534	VAL	3.4
1	F	558	ALA	3.4
1	C	327	MET	3.4
1	C	485	THR	3.4
1	A	442	HIS	3.4
1	F	474	HIS	3.4
1	C	430	LEU	3.4
1	C	532	ARG	3.3
1	D	295	GLY	3.3
1	C	316	PHE	3.3
1	F	443	GLN	3.3
1	B	199	ASP	3.3
1	C	422	SER	3.3
1	F	292	SER	3.3
1	F	548	GLY	3.3
1	C	503	ALA	3.3
1	C	568	ASN	3.3
1	C	111	LYS	3.3
1	C	146	ASN	3.2
1	C	391	GLU	3.2
1	F	513	CYS	3.2
1	C	550	LEU	3.2
1	C	288	GLU	3.2
1	A	540	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	131	TRP	3.2
1	C	145	HIS	3.2
1	F	465	ASP	3.1
1	C	262	GLN	3.1
1	B	94	SER	3.1
1	A	128	ARG	3.1
1	C	181	PRO	3.1
1	C	525	ILE	3.1
1	C	385	ALA	3.1
1	C	186	LEU	3.1
1	C	292	SER	3.1
1	C	397	TYR	3.0
1	C	472	GLU	3.0
1	B	96	GLN	3.0
1	F	493	MET	3.0
1	C	506	SER	3.0
1	D	130	GLN	3.0
1	E	93	ARG	3.0
1	C	557	PRO	3.0
1	F	284	TYR	3.0
1	C	537	ASN	3.0
1	C	518	SER	2.9
1	C	277	ASN	2.9
1	C	390	ASP	2.9
1	C	328	MET	2.9
1	F	288	GLU	2.9
1	A	95	GLY	2.9
1	C	124	ASP	2.9
1	C	286	THR	2.9
1	C	91	MET	2.9
1	C	449	ALA	2.9
1	C	275	ASP	2.9
1	C	501	ASP	2.9
1	C	543	ARG	2.9
1	D	450	LEU	2.9
1	D	540	LEU	2.9
1	B	127	GLN	2.9
1	F	486	LYS	2.9
1	F	286	THR	2.9
1	F	457	LEU	2.9
1	C	416	GLU	2.8
1	F	526	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	284	TYR	2.8
1	B	457	LEU	2.8
1	F	97	ASP	2.8
1	F	441	ASP	2.8
1	A	93	ARG	2.8
1	F	545	ALA	2.8
1	C	108	GLU	2.8
1	E	442	HIS	2.8
1	C	291	ARG	2.8
1	F	500	VAL	2.7
1	F	550	LEU	2.7
1	C	526	GLU	2.7
1	C	402	SER	2.7
1	C	386	GLU	2.7
1	D	457	LEU	2.7
1	C	426	PHE	2.7
1	C	425	PRO	2.7
1	A	409	GLY	2.7
1	C	535	GLY	2.7
1	D	531	LEU	2.7
1	F	450	LEU	2.7
1	D	290	ARG	2.7
1	D	296	ASN	2.7
1	C	290	ARG	2.7
1	C	387	VAL	2.7
1	F	487	GLU	2.7
1	F	199	ASP	2.7
1	C	380	ASN	2.6
1	C	404	ARG	2.6
1	D	288	GLU	2.6
1	A	419	LYS	2.6
1	F	384	ALA	2.6
1	F	391	GLU	2.6
1	B	442	HIS	2.6
1	C	549	GLY	2.6
1	C	278	LEU	2.6
1	C	428	TRP	2.6
1	F	463	PHE	2.6
1	C	362	ARG	2.6
1	C	469	GLY	2.6
1	E	540	LEU	2.6
1	F	363	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	X	5	SER	2.6
1	B	295	GLY	2.6
1	C	409	GLY	2.6
1	C	545	ALA	2.6
1	F	566	THR	2.6
1	C	563	TRP	2.5
1	F	505	GLY	2.5
1	C	295	GLY	2.5
1	C	388	TRP	2.5
1	B	128	ARG	2.5
1	F	179	ASN	2.5
1	C	491	LYS	2.5
1	C	431	GLU	2.5
1	F	243	GLU	2.5
1	F	291	ARG	2.4
1	C	157	VAL	2.4
1	F	502	ARG	2.4
1	D	442	HIS	2.4
1	C	325	ASP	2.4
1	F	419	LYS	2.4
1	A	316	PHE	2.4
1	A	290	ARG	2.4
1	D	293	ARG	2.4
1	C	478	GLY	2.4
1	E	95	GLY	2.4
1	C	429	TYR	2.4
1	F	368	THR	2.4
2	Y	5	SER	2.3
2	Y	8	PRO	2.3
1	F	295	GLY	2.3
1	C	414	ARG	2.3
1	C	395	PHE	2.3
1	D	199	ASP	2.3
1	C	389	MET	2.3
1	F	471	TYR	2.3
1	F	517	ASP	2.3
1	A	454	THR	2.3
1	B	288	GLU	2.3
1	F	518	SER	2.3
1	C	470	VAL	2.3
1	D	294	GLN	2.3
1	F	538	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	490	VAL	2.3
1	C	382	ARG	2.2
1	C	553	GLU	2.2
1	E	316	PHE	2.2
1	B	130	GLN	2.2
1	C	76	VAL	2.2
1	C	324	TYR	2.2
1	C	564	LYS	2.2
1	C	565	PHE	2.2
1	C	258	MET	2.2
1	C	245	ARG	2.2
1	C	344	GLN	2.2
1	C	287	PRO	2.2
1	C	178	SER	2.2
1	C	529	SER	2.2
1	E	94	SER	2.2
1	C	338	ILE	2.2
1	F	470	VAL	2.2
1	C	451	GLN	2.2
1	B	540	LEU	2.2
1	E	419	LYS	2.1
1	F	507	LEU	2.1
1	C	307	ALA	2.1
1	C	556	GLY	2.1
1	C	87	VAL	2.1
1	C	296	ASN	2.1
1	F	473	CYS	2.1
1	D	475	ASN	2.1
1	C	156	VAL	2.1
1	E	128	ARG	2.1
1	C	337	GLU	2.1
1	C	450	LEU	2.1
1	C	125	GLN	2.1
1	C	420	LYS	2.1
1	A	130	GLN	2.0
1	C	517	ASP	2.0
1	A	422	SER	2.0
1	C	435	PRO	2.0
1	F	200	ARG	2.0
1	A	443	GLN	2.0
1	C	345	CYS	2.0
1	C	462	HIS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	A	1577	4/4	0.85	0.49	11.59	62,68,71,76	0
5	BBK	E	1584	15/15	0.70	0.32	7.72	96,105,117,124	0
5	BBK	D	1572	15/15	0.65	0.32	7.20	96,105,117,124	0
5	BBK	B	1580	15/15	0.63	0.29	7.05	69,86,120,142	0
4	EDO	A	1573	4/4	0.83	0.20	4.87	56,68,70,70	0
4	EDO	E	1570	4/4	0.81	0.32	4.64	44,48,59,61	0
4	EDO	A	1576	4/4	0.88	0.26	4.56	57,62,66,75	0
4	EDO	B	1573	4/4	0.88	0.27	4.53	40,41,42,48	0
4	EDO	A	1580	4/4	0.80	0.23	3.93	45,52,57,59	0
4	EDO	A	1579	4/4	0.85	0.18	3.49	51,52,54,64	0
4	EDO	E	1577	4/4	0.94	0.21	2.97	61,61,64,68	0
4	EDO	A	1574	4/4	0.89	0.15	2.56	51,52,54,57	0
4	EDO	B	1578	4/4	0.90	0.28	2.15	55,58,62,69	0
4	EDO	E	1572	4/4	0.91	0.25	2.00	38,45,48,51	0
4	EDO	A	1571	4/4	0.94	0.21	2.00	43,46,46,52	0
4	EDO	A	1572	4/4	0.82	0.24	1.75	57,66,67,69	0
4	EDO	E	1581	4/4	0.91	0.17	1.62	53,56,60,68	0
4	EDO	D	1573	4/4	0.91	0.14	1.58	38,40,40,45	0
4	EDO	D	1576	4/4	0.94	0.15	1.49	39,43,45,49	0
4	EDO	B	1577	4/4	0.94	0.20	1.37	42,43,48,57	0
4	EDO	E	1583	4/4	0.91	0.15	1.28	58,61,62,68	0
5	BBK	A	1581	15/15	0.78	0.23	1.05	69,86,120,142	0
4	EDO	A	1578	4/4	0.92	0.18	1.04	38,45,48,63	0
4	EDO	D	1575	4/4	0.64	0.22	0.81	60,63,68,70	0
4	EDO	B	1579	4/4	0.90	0.13	0.66	41,48,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	HWU	F	1571	39/39	0.91	0.12	0.18	38,44,55,60	0
4	EDO	E	1574	4/4	0.81	0.19	0.17	62,68,68,75	0
4	EDO	E	1582	4/4	0.96	0.12	0.01	47,48,51,56	0
4	EDO	A	1575	4/4	0.96	0.11	-0.01	53,55,57,59	0
4	EDO	E	1571	4/4	0.96	0.17	-0.04	38,46,47,50	0
6	HWU	B	1571	39/39	0.92	0.13	-0.13	30,36,44,49	0
4	EDO	E	1575	4/4	0.80	0.16	-0.14	64,69,69,76	0
6	HWU	A	1582	39/39	0.92	0.12	-0.14	26,34,45,48	0
4	EDO	B	1572	4/4	0.95	0.10	-0.19	34,35,35,42	0
6	HWU	D	1571	39/39	0.93	0.12	-0.21	24,35,45,46	0
6	HWU	E	1585	39/39	0.95	0.12	-0.32	26,36,54,58	0
4	EDO	B	1574	4/4	0.95	0.10	-0.48	40,40,42,45	0
6	HWU	C	1569	39/39	0.86	0.18	-0.54	51,76,89,92	0
4	EDO	E	1579	4/4	0.96	0.11	-0.62	43,44,52,53	0
4	EDO	E	1573	4/4	0.90	0.22	-	49,58,60,71	0
4	EDO	B	1576	4/4	0.74	0.24	-	65,69,73,76	0
3	MN	A	1570	1/1	0.99	0.08	-	27,27,27,27	0
4	EDO	D	1574	4/4	0.91	0.12	-	49,50,52,58	0
3	MN	B	1570	1/1	1.00	0.09	-	33,33,33,33	0
4	EDO	E	1576	4/4	0.87	0.19	-	68,68,69,69	0
3	MN	E	1586	1/1	0.99	0.08	-	26,26,26,26	0
3	MN	C	1570	1/1	0.95	0.04	-	59,59,59,59	0
4	EDO	B	1575	4/4	0.93	0.25	-	66,68,69,69	0
4	EDO	E	1578	4/4	0.89	0.23	-	64,64,66,82	0
4	EDO	D	1577	4/4	0.85	0.20	-	67,68,69,69	0
4	EDO	E	1580	4/4	0.78	0.31	-	59,70,71,76	0
3	MN	F	1570	1/1	1.00	0.03	-	42,42,42,42	0
3	MN	D	1570	1/1	1.00	0.08	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.