Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:02 AM GMT

PDB ID	:	3KLZ
Title	:	Pentameric formate channel with formate bound
Authors	:	Waight, A.B.; Wang, D.N.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on	:	2009-11-09
Resolution	:	2.50 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 ①) were used in the production of this report:

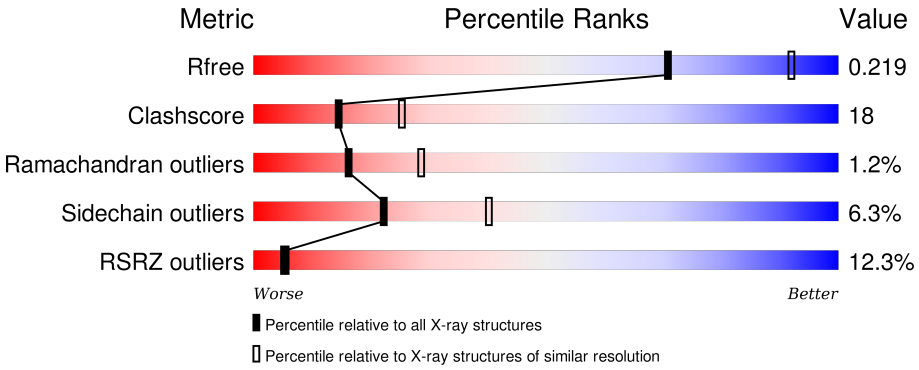
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	280	9% 67% 21% • • 8%
1	B	280	11% 65% 22% 5% 9%
1	C	280	12% 65% 25% • 9%
1	D	280	14% 64% 24% • 9%
1	E	280	11% 69% 20% • 8%

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	BOG	A	281	-	-	-	X
2	BOG	A	282	X	-	-	X
2	BOG	B	281	-	-	-	X
2	BOG	B	282	-	-	-	X
2	BOG	B	283	-	-	X	X
2	BOG	B	284	-	-	-	X
2	BOG	B	285	-	-	X	X
2	BOG	B	286	-	-	-	X
2	BOG	C	281	-	-	-	X
2	BOG	C	282	-	-	-	X
2	BOG	D	281	-	-	-	X
2	BOG	E	281	-	-	-	X
3	FMT	A	284	-	-	-	X
3	FMT	A	285	-	-	X	X
3	FMT	A	286	-	-	-	X
3	FMT	A	292	-	-	-	X
3	FMT	B	287	-	-	-	X
3	FMT	B	288	-	-	-	X
3	FMT	B	290	-	-	X	-
3	FMT	B	291	-	-	-	X
3	FMT	B	292	-	-	-	X
3	FMT	B	294	-	-	-	X
3	FMT	B	295	-	-	-	X
3	FMT	C	283	-	-	X	X
3	FMT	C	284	-	-	-	X
3	FMT	D	283	-	-	-	X
3	FMT	D	288	-	-	-	X
3	FMT	E	283	-	-	-	X
3	FMT	E	285	-	-	-	X
3	FMT	E	286	-	-	-	X
3	FMT	E	311	-	-	-	X
3	FMT	E	312	-	-	X	-

2 Entry composition

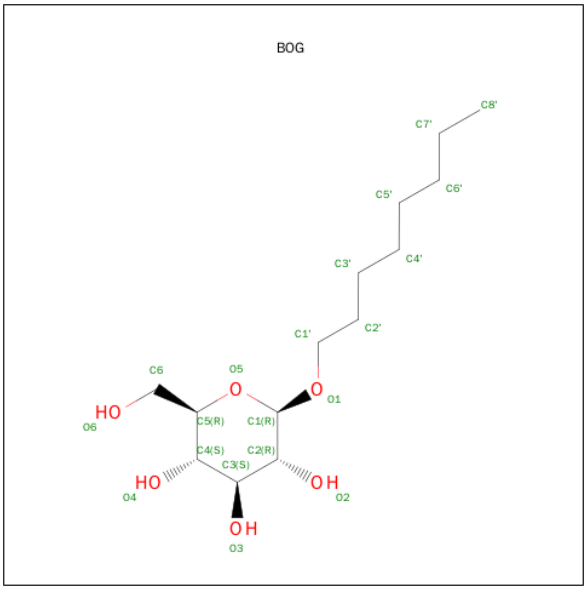
There are 4 unique types of molecules in this entry. The entry contains 10446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 formate transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1973	1313	312	332	16			
1	B	256	Total	C	N	O	S	0	0	0
			1962	1307	310	329	16			
1	C	255	Total	C	N	O	S	0	0	0
			1958	1306	310	326	16			
1	D	255	Total	C	N	O	S	0	0	0
			1958	1306	310	326	16			
1	E	257	Total	C	N	O	S	0	0	0
			1971	1313	312	330	16			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		

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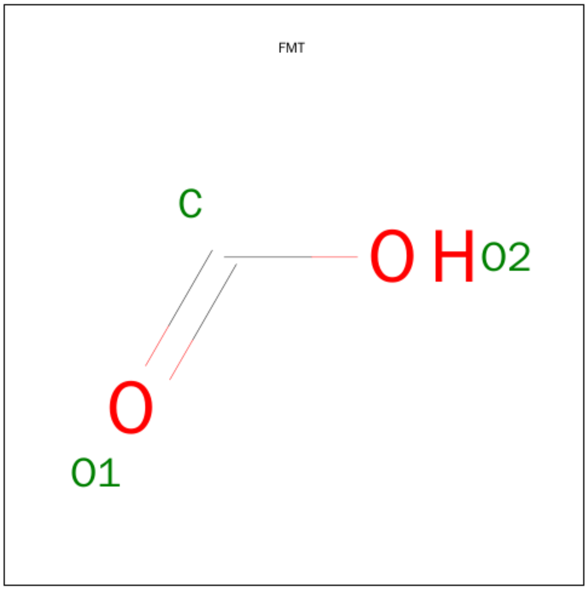
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 20 14 6	0	0
2	A	1	Total C O 20 14 6	0	0
2	B	1	Total C O 20 14 6	0	0
2	B	1	Total C O 20 14 6	0	0
2	B	1	Total C O 20 14 6	0	0
2	B	1	Total C O 20 14 6	0	0
2	B	1	Total C O 20 14 6	0	0
2	B	1	Total C O 20 14 6	0	0
2	C	1	Total C O 20 14 6	0	0
2	C	1	Total C O 20 14 6	0	0
2	D	1	Total C O 20 14 6	0	0
2	E	1	Total C O 20 14 6	0	0
2	E	1	Total C O 20 14 6	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0

- Molecule 4 is water.

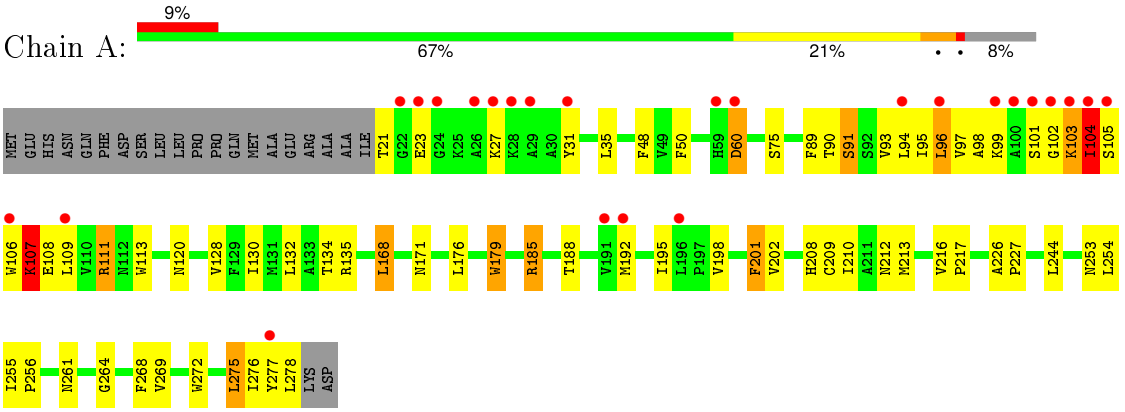
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	61	Total O 61 61	0	0
4	C	45	Total O 45 45	0	0
4	D	30	Total O 30 30	0	0
4	E	35	Total O 35 35	0	0

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.

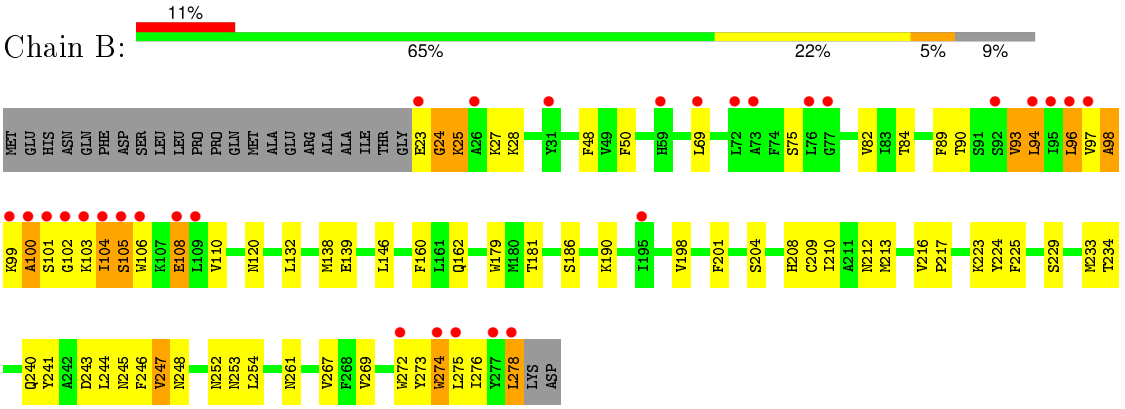
- Molecule 1: Putative formate transporter 1

Chain A:



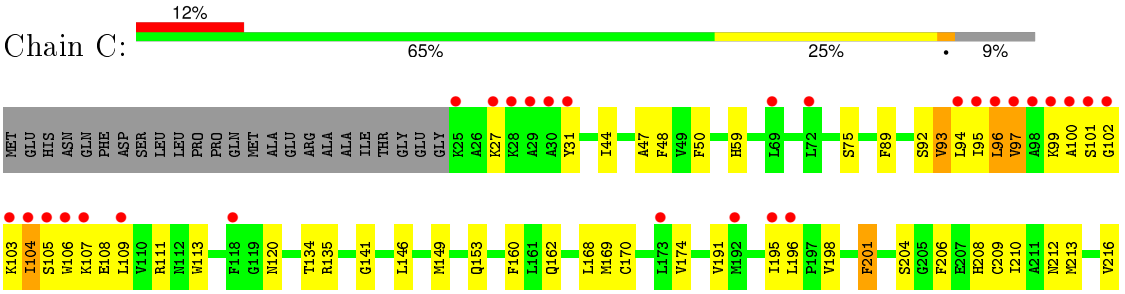
- Molecule 1: Putative formate transporter 1

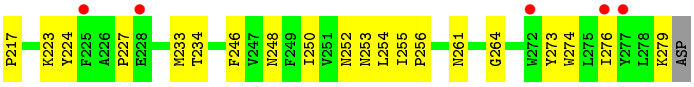
Chain B:



- Molecule 1: Putative formate transporter 1

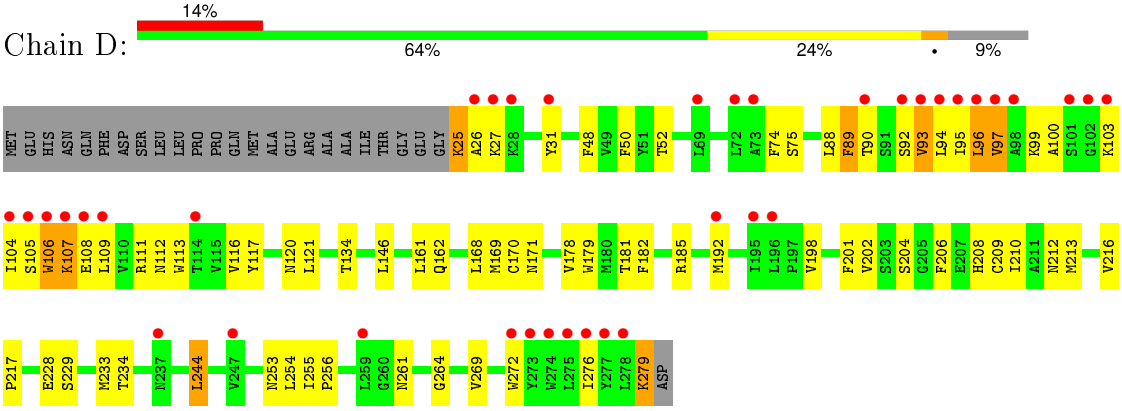
Chain C:





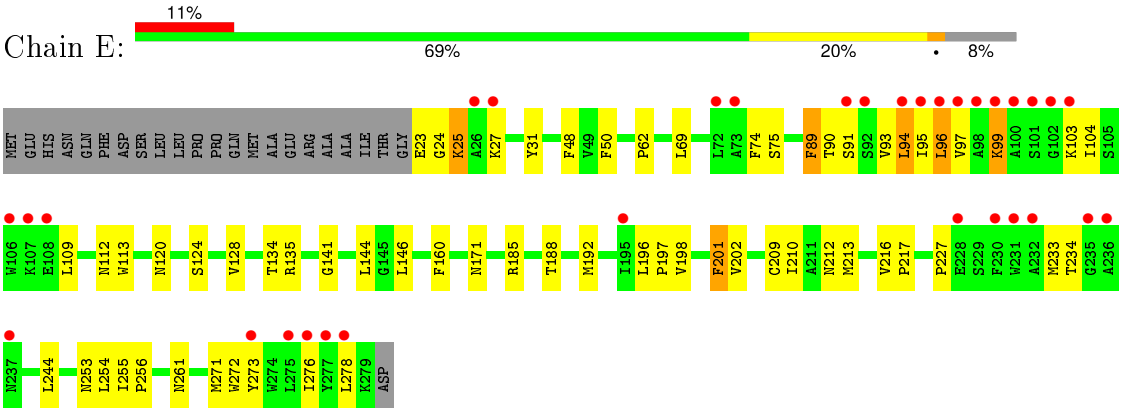
- Molecule 1: Putative formate transporter 1

Chain D:



- Molecule 1: Putative formate transporter 1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.78Å 100.46Å 192.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.50 48.24 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.24-2.50) 94.5 (48.24-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.173 , 0.223 0.172 , 0.219	Depositor DCC
R_{free} test set	1921 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.1	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 64102 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10446	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: FMT, BOG

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	0.44	0/2021	0.52	1/2744 (0.0%)
1	B	0.44	0/2010	0.53	0/2729
1	C	0.42	0/2006	0.50	0/2723
1	D	0.37	0/2006	0.47	0/2723
1	E	0.39	0/2019	0.49	0/2740
All	All	0.41	0/10062	0.50	1/13659 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1973	0	2035	76	0
1	B	1962	0	2025	91	0
1	C	1958	0	2029	68	0
1	D	1958	0	2029	78	0
1	E	1971	0	2038	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	60	0	82	11	0
2	B	120	0	167	39	0
2	C	40	0	55	4	0
2	D	20	0	28	4	0
2	E	40	0	56	7	0
3	A	27	0	9	3	0
3	B	27	0	9	4	0
3	C	18	0	6	3	0
3	D	21	0	7	2	0
3	E	24	0	8	2	0
4	A	56	0	0	1	0
4	B	61	0	0	0	0
4	C	45	0	0	1	0
4	D	30	0	0	3	0
4	E	35	0	0	0	0
All	All	10446	0	10583	372	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 18.

All (372) 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:D:105:SER:H	1:D:106:TRP:HA	1.10	1.08
1:B:24:GLY:HA2	1:B:27:LYS:CB	1.87	1.04
1:A:97:VAL:H	1:A:98:ALA:HB3	1.24	1.00
1:B:104:ILE:HB	1:B:108:GLU:HB2	1.43	1.00
1:B:89:PHE:H	1:B:120:ASN:HD21	1.03	0.96
1:C:89:PHE:H	1:C:120:ASN:HD21	1.14	0.95
1:E:89:PHE:H	1:E:120:ASN:HD21	1.11	0.94
1:E:95:ILE:HG21	1:E:112:ASN:HD22	1.33	0.94
1:B:24:GLY:HA2	1:B:27:LYS:HB3	1.49	0.91
2:A:282:BOG:O2	2:A:282:BOG:H2'1	1.72	0.90
1:C:104:ILE:HG13	1:C:108:GLU:H	1.35	0.89
1:B:24:GLY:HA2	1:B:27:LYS:HB2	1.53	0.89
1:D:89:PHE:H	1:D:120:ASN:HD21	1.13	0.89
1:D:105:SER:HB3	1:D:108:GLU:H	1.39	0.87
1:B:246:PHE:H	2:B:283:BOG:H5'1	1.36	0.87
1:C:135:ARG:HD2	3:C:283:FMT:H	1.56	0.87
1:D:103:LYS:HB3	1:D:104:ILE:HA	1.56	0.86
1:E:209:CYS:H	1:E:261:ASN:HD21	1.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:VAL:HG23	1:D:116:VAL:HG21	1.57	0.85
1:A:97:VAL:N	1:A:98:ALA:HB3	1.90	0.84
1:A:195:ILE:HG21	2:A:282:BOG:O3	1.77	0.84
1:D:105:SER:N	1:D:106:TRP:HA	1.85	0.84
1:D:229:SER:O	1:D:233:MET:HG2	1.77	0.83
1:A:89:PHE:H	1:A:120:ASN:HD21	1.26	0.81
1:B:212:ASN:HD22	1:B:253:ASN:HD21	1.29	0.80
1:D:212:ASN:HD22	1:D:253:ASN:HD21	1.27	0.80
1:B:209:CYS:H	1:B:261:ASN:HD21	1.26	0.80
1:B:89:PHE:H	1:B:120:ASN:ND2	1.80	0.79
2:A:282:BOG:O2	2:A:282:BOG:C2'	2.30	0.79
2:A:282:BOG:O2	2:A:282:BOG:C1'	2.30	0.79
1:C:255:ILE:HB	1:C:256:PRO:HD3	1.65	0.78
1:D:93:VAL:HG11	1:D:113:TRP:HE1	1.48	0.78
1:A:176:LEU:HD21	2:A:281:BOG:H6'2	1.65	0.78
1:B:190:LYS:NZ	2:B:285:BOG:H5	1.97	0.78
1:D:89:PHE:H	1:D:120:ASN:ND2	1.83	0.77
1:C:96:LEU:HD13	1:C:97:VAL:H	1.48	0.77
1:A:91:SER:O	1:A:94:LEU:HG	1.85	0.76
1:E:89:PHE:H	1:E:120:ASN:ND2	1.82	0.76
1:C:89:PHE:H	1:C:120:ASN:ND2	1.85	0.75
1:A:209:CYS:H	1:A:261:ASN:HD21	1.32	0.75
1:B:245:ASN:HB2	2:B:283:BOG:H4'2	1.70	0.74
1:D:94:LEU:HB3	1:D:97:VAL:HG11	1.70	0.73
1:B:247:VAL:HG13	2:B:283:BOG:C1'	2.18	0.73
2:A:282:BOG:H1'2	2:A:282:BOG:O2	1.90	0.71
1:B:190:LYS:CE	2:B:285:BOG:H5	2.21	0.71
1:C:104:ILE:HG13	1:C:108:GLU:N	2.07	0.69
1:A:75:SER:HA	1:A:198:VAL:HG11	1.75	0.69
1:D:89:PHE:N	1:D:120:ASN:HD21	1.90	0.69
1:D:93:VAL:HG21	1:D:113:TRP:HD1	1.57	0.69
1:B:247:VAL:HG13	2:B:283:BOG:H1'2	1.75	0.69
1:A:93:VAL:O	1:A:96:LEU:HD22	1.93	0.68
1:A:104:ILE:HG13	1:A:105:SER:HA	1.75	0.67
1:D:90:THR:HG23	4:D:318:HOH:O	1.93	0.67
2:B:286:BOG:H2'2	2:B:286:BOG:O5	1.95	0.66
1:B:190:LYS:HZ1	2:B:285:BOG:H5	1.57	0.66
1:A:89:PHE:H	1:A:120:ASN:ND2	1.94	0.66
1:D:93:VAL:HG22	1:D:112:ASN:HD21	1.59	0.66
1:B:246:PHE:HD2	2:B:283:BOG:H5'2	1.60	0.66
1:E:255:ILE:HB	1:E:256:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:VAL:O	1:E:97:VAL:HG13	1.97	0.65
1:D:100:ALA:HA	1:D:103:LYS:O	1.96	0.64
1:C:168:LEU:CD1	1:C:264:GLY:HA2	2.27	0.64
1:C:196:LEU:HD21	2:C:281:BOG:H1'1	1.80	0.64
1:D:88:LEU:H	1:D:92:SER:HB2	1.64	0.63
1:B:23:GLU:O	1:B:25:LYS:N	2.29	0.63
1:D:255:ILE:HB	1:D:256:PRO:HD3	1.79	0.63
1:B:69:LEU:HD21	2:B:282:BOG:H8'3	1.80	0.63
1:B:24:GLY:CA	1:B:27:LYS:HB3	2.25	0.63
1:A:185:ARG:O	1:A:185:ARG:HD3	1.97	0.63
1:D:120:ASN:HB3	1:D:210:ILE:HG23	1.81	0.63
1:B:139:GLU:HG3	3:B:287:FMT:H	1.81	0.62
1:C:135:ARG:HD2	3:C:283:FMT:C	2.29	0.62
1:B:209:CYS:H	1:B:261:ASN:ND2	1.96	0.62
1:A:99:LYS:HD2	1:A:109:LEU:HD13	1.79	0.62
1:D:93:VAL:HG21	1:D:113:TRP:CD1	2.34	0.62
1:B:138:MET:HB3	3:B:290:FMT:H	1.82	0.62
1:E:93:VAL:HA	1:E:96:LEU:HD22	1.82	0.62
1:D:209:CYS:H	1:D:261:ASN:HD21	1.47	0.61
1:D:90:THR:O	1:D:93:VAL:HG12	2.01	0.61
1:D:99:LYS:NZ	1:D:103:LYS:HG2	2.15	0.61
1:D:95:ILE:HG21	1:D:269:VAL:HG21	1.82	0.61
1:B:190:LYS:HZ1	2:B:285:BOG:C5	2.13	0.61
1:C:93:VAL:HA	1:C:96:LEU:HB2	1.83	0.61
2:C:281:BOG:H3	2:D:281:BOG:C6	2.31	0.61
1:C:209:CYS:H	1:C:261:ASN:HD21	1.49	0.61
1:A:195:ILE:HB	2:A:282:BOG:O6	2.01	0.61
1:D:103:LYS:HE3	1:D:104:ILE:HA	1.83	0.60
1:A:106:TRP:O	1:A:108:GLU:N	2.32	0.60
2:C:281:BOG:H3	2:D:281:BOG:H61	1.83	0.60
1:C:108:GLU:HA	1:C:111:ARG:HB3	1.84	0.60
1:A:97:VAL:HG22	1:A:269:VAL:HG13	1.83	0.60
1:E:141:GLY:HA2	1:E:233:MET:CE	2.31	0.60
1:A:102:GLY:H	1:A:103:LYS:HG3	1.66	0.59
1:D:75:SER:HA	1:D:198:VAL:HG11	1.84	0.59
1:D:279:LYS:HB2	1:D:279:LYS:NZ	2.18	0.59
1:A:212:ASN:HD22	1:A:253:ASN:HD21	1.49	0.58
1:C:111:ARG:HH11	1:C:111:ARG:HA	1.67	0.58
1:B:247:VAL:H	2:B:283:BOG:H3'1	1.67	0.58
1:A:202:VAL:O	3:A:292:FMT:H	2.04	0.58
1:A:185:ARG:C	1:A:185:ARG:HD3	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HD12	1:A:109:LEU:HB2	1.86	0.57
1:A:101:SER:HB2	1:A:102:GLY:HA2	1.85	0.57
1:E:99:LYS:HG3	1:E:109:LEU:HB2	1.86	0.57
1:C:93:VAL:HG12	1:C:96:LEU:HG	1.85	0.57
1:C:168:LEU:HD12	1:C:264:GLY:HA2	1.86	0.57
1:A:255:ILE:HB	1:A:256:PRO:HD3	1.87	0.57
1:A:21:THR:HG22	1:A:23:GLU:H	1.69	0.57
1:E:95:ILE:HG13	1:E:112:ASN:ND2	2.20	0.56
1:E:89:PHE:N	1:E:120:ASN:HD21	1.93	0.56
1:D:93:VAL:HG11	1:D:113:TRP:NE1	2.19	0.56
1:E:209:CYS:H	1:E:261:ASN:ND2	2.00	0.56
1:C:108:GLU:HA	1:C:111:ARG:CB	2.36	0.56
1:B:274:TRP:HA	1:B:274:TRP:CE3	2.39	0.56
1:D:89:PHE:O	1:D:93:VAL:HB	2.04	0.56
1:A:94:LEU:HA	1:A:269:VAL:HG21	1.88	0.56
2:A:282:BOG:C2	2:A:282:BOG:H2'1	2.35	0.56
1:C:75:SER:HA	1:C:198:VAL:HG11	1.87	0.56
1:A:120:ASN:HB3	1:A:210:ILE:HG23	1.88	0.56
1:B:190:LYS:HE3	2:B:285:BOG:H1	1.88	0.56
3:A:285:FMT:H	1:E:62:PRO:HA	1.88	0.56
1:C:101:SER:HB3	1:C:109:LEU:HG	1.88	0.56
1:E:69:LEU:HD21	2:E:281:BOG:H7'2	1.88	0.56
1:D:272:TRP:O	1:D:276:ILE:HG12	2.05	0.56
1:D:25:LYS:HG3	1:D:27:LYS:H	1.69	0.56
1:B:190:LYS:HZ1	2:B:285:BOG:H1	1.72	0.55
1:D:89:PHE:HB3	3:D:282:FMT:O1	2.06	0.55
1:A:97:VAL:CA	1:A:98:ALA:HB3	2.35	0.55
1:B:246:PHE:HB2	2:B:283:BOG:H3'2	1.88	0.55
1:C:27:LYS:HE3	1:C:31:TYR:HE2	1.71	0.55
1:B:229:SER:O	1:B:233:MET:HG2	2.06	0.55
1:C:212:ASN:HD22	1:C:253:ASN:HD21	1.55	0.54
1:C:250:ILE:O	1:C:255:ILE:HG12	2.06	0.54
1:A:277:TYR:O	1:A:278:LEU:HB2	2.06	0.54
1:C:104:ILE:H	1:C:104:ILE:HD13	1.71	0.54
1:E:120:ASN:HB3	1:E:210:ILE:HG23	1.88	0.54
1:B:246:PHE:N	2:B:283:BOG:H5'1	2.15	0.54
1:A:209:CYS:H	1:A:261:ASN:ND2	2.04	0.54
1:B:96:LEU:O	1:B:101:SER:HA	2.08	0.54
1:A:104:ILE:HG22	1:A:108:GLU:HB3	1.88	0.54
1:A:27:LYS:HG2	1:A:31:TYR:CE2	2.42	0.54
1:B:246:PHE:HD2	2:B:283:BOG:C5'	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:H	2:B:283:BOG:C3'	2.20	0.54
1:A:97:VAL:HB	1:A:98:ALA:CB	2.38	0.53
3:A:285:FMT:C	1:E:62:PRO:HA	2.38	0.53
1:B:99:LYS:O	1:B:100:ALA:HB3	2.07	0.53
1:D:209:CYS:H	1:D:261:ASN:ND2	2.06	0.53
1:A:102:GLY:N	1:A:103:LYS:HG3	2.24	0.53
1:D:90:THR:HA	1:D:93:VAL:HB	1.91	0.53
1:E:99:LYS:HG2	1:E:104:ILE:HG13	1.90	0.53
1:D:99:LYS:HZ1	1:D:103:LYS:HG2	1.74	0.53
1:A:101:SER:N	1:A:102:GLY:HA2	2.24	0.53
1:A:60:ASP:OD1	1:A:60:ASP:N	2.34	0.53
1:C:111:ARG:HA	1:C:111:ARG:NH1	2.24	0.53
1:C:96:LEU:HD13	1:C:97:VAL:N	2.21	0.53
1:B:75:SER:HA	1:B:198:VAL:HG11	1.90	0.53
1:C:107:LYS:HB3	1:C:107:LYS:NZ	2.24	0.53
1:A:97:VAL:HG22	1:A:269:VAL:HG22	1.91	0.52
1:B:247:VAL:HG22	2:B:283:BOG:H3'1	1.90	0.52
1:E:25:LYS:NZ	1:E:25:LYS:HB2	2.25	0.52
1:E:90:THR:HG21	2:E:310:BOG:C8'	2.39	0.52
1:B:106:TRP:O	1:B:110:VAL:HG22	2.09	0.52
1:E:212:ASN:HD22	1:E:253:ASN:HD21	1.57	0.52
1:E:216:VAL:HB	1:E:217:PRO:HD3	1.92	0.52
1:B:245:ASN:HD21	2:B:286:BOG:H1'2	1.75	0.52
1:E:27:LYS:O	1:E:31:TYR:HD2	1.92	0.52
1:C:246:PHE:HE2	2:C:282:BOG:H3'2	1.75	0.52
1:B:190:LYS:HZ1	2:B:285:BOG:C1	2.22	0.52
1:C:149:MET:O	1:C:153:GLN:HG3	2.10	0.52
1:B:224:TYR:CE2	2:B:283:BOG:H8'3	2.45	0.52
1:D:93:VAL:HG22	1:D:112:ASN:ND2	2.24	0.52
1:B:97:VAL:HG13	1:B:98:ALA:H	1.74	0.51
1:D:103:LYS:CB	1:D:104:ILE:HA	2.27	0.51
1:E:27:LYS:HZ2	1:E:31:TYR:HE2	1.56	0.51
1:B:190:LYS:HZ3	2:B:285:BOG:C6'	2.23	0.51
1:C:107:LYS:HB3	1:C:107:LYS:HZ3	1.76	0.51
1:B:146:LEU:HD11	1:B:234:THR:HB	1.92	0.51
1:B:23:GLU:C	1:B:25:LYS:H	2.13	0.51
1:E:103:LYS:HG3	1:E:104:ILE:HG23	1.92	0.51
1:E:90:THR:HG22	1:E:113:TRP:CZ2	2.45	0.51
1:E:90:THR:HG21	2:E:310:BOG:H8'1	1.93	0.51
1:B:101:SER:HB3	1:B:105:SER:HA	1.92	0.51
1:E:94:LEU:O	1:E:97:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:O	1:A:192:MET:HG2	2.11	0.50
1:B:245:ASN:HB2	2:B:283:BOG:C4'	2.39	0.50
1:C:191:VAL:O	1:C:195:ILE:HG13	2.11	0.50
1:D:27:LYS:O	1:D:31:TYR:HD2	1.95	0.50
1:D:146:LEU:HD11	1:D:234:THR:HB	1.93	0.49
1:C:273:TYR:O	1:C:276:ILE:HG13	2.11	0.49
1:C:92:SER:C	1:C:94:LEU:H	2.16	0.49
1:D:108:GLU:HA	1:D:111:ARG:HB3	1.94	0.49
1:B:190:LYS:HZ3	2:B:285:BOG:H6'2	1.78	0.49
1:A:96:LEU:HA	1:A:99:LYS:HB2	1.95	0.49
1:B:240:GLN:O	3:B:292:FMT:H	2.12	0.49
1:B:93:VAL:HG22	1:B:269:VAL:HG21	1.93	0.49
3:E:311:FMT:H	3:E:312:FMT:C	2.43	0.49
1:E:124:SER:O	1:E:128:VAL:HG23	2.12	0.49
1:D:168:LEU:HD12	1:D:264:GLY:HA2	1.94	0.49
1:B:233:MET:HE1	3:B:290:FMT:C	2.42	0.49
1:D:27:LYS:HE3	1:D:31:TYR:HE2	1.76	0.48
1:B:224:TYR:HE2	2:B:283:BOG:H8'3	1.78	0.48
1:A:96:LEU:HB3	1:A:109:LEU:HD11	1.95	0.48
1:D:179:TRP:CE3	1:D:182:PHE:HD2	2.31	0.48
1:C:104:ILE:HG21	1:C:108:GLU:HB2	1.94	0.48
1:A:103:LYS:NZ	1:A:103:LYS:HB2	2.29	0.48
1:E:23:GLU:HG2	1:E:24:GLY:H	1.79	0.48
1:C:216:VAL:HB	1:C:217:PRO:HD3	1.96	0.48
1:A:99:LYS:HD2	1:A:109:LEU:CD1	2.44	0.48
1:C:99:LYS:HB3	1:C:99:LYS:NZ	2.29	0.48
1:D:27:LYS:HE3	1:D:31:TYR:CE2	2.48	0.48
1:E:23:GLU:HG2	1:E:24:GLY:N	2.29	0.48
1:A:216:VAL:HB	1:A:217:PRO:HD3	1.96	0.47
1:A:272:TRP:NE1	1:A:276:ILE:HD11	2.29	0.47
1:E:75:SER:HA	1:E:198:VAL:HG11	1.94	0.47
2:A:282:BOG:H6'1	2:B:282:BOG:H6'2	1.97	0.47
1:A:208:HIS:CE1	1:A:210:ILE:HB	2.49	0.47
1:D:27:LYS:HG3	1:D:31:TYR:HE2	1.79	0.47
1:C:105:SER:C	1:C:107:LYS:H	2.18	0.47
1:A:90:THR:HB	1:A:171:ASN:OD1	2.14	0.47
1:C:169:MET:HB3	1:C:206:PHE:CE2	2.49	0.47
1:B:104:ILE:HD12	1:B:108:GLU:CG	2.45	0.47
1:D:93:VAL:CG2	1:D:116:VAL:HG21	2.36	0.47
1:C:96:LEU:HD22	1:C:109:LEU:HD21	1.96	0.47
1:C:209:CYS:H	1:C:261:ASN:ND2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:HD23	1:E:144:LEU:O	2.15	0.47
1:E:272:TRP:O	1:E:276:ILE:HG12	2.14	0.47
1:B:246:PHE:H	2:B:283:BOG:C5'	2.16	0.47
1:B:181:THR:OG1	2:B:285:BOG:H8'1	2.15	0.47
1:C:223:LYS:HE2	1:C:224:TYR:CZ	2.49	0.47
1:B:273:TYR:O	1:B:276:ILE:HG13	2.15	0.47
1:B:179:TRP:HH2	1:B:272:TRP:CZ2	2.33	0.47
1:A:109:LEU:HD21	1:A:113:TRP:CE2	2.50	0.46
1:B:23:GLU:O	1:B:23:GLU:HG3	2.15	0.46
1:B:190:LYS:CE	2:B:285:BOG:H1	2.45	0.46
1:A:101:SER:HB2	1:A:102:GLY:CA	2.46	0.46
1:D:93:VAL:O	1:D:94:LEU:HB2	2.16	0.46
1:C:44:ILE:O	1:C:47:ALA:HB3	2.15	0.46
1:B:223:LYS:HD2	1:B:241:TYR:HB2	1.96	0.46
1:E:91:SER:HB3	1:E:112:ASN:ND2	2.30	0.46
1:D:208:HIS:CE1	1:D:210:ILE:HB	2.50	0.46
1:C:141:GLY:HA2	1:C:233:MET:CE	2.45	0.46
2:E:310:BOG:H1	3:E:312:FMT:O2	2.16	0.46
1:D:253:ASN:O	1:D:256:PRO:HD2	2.16	0.46
1:B:213:MET:O	1:B:217:PRO:HG2	2.15	0.46
2:D:281:BOG:O5	2:E:281:BOG:H61	2.16	0.45
1:B:278:LEU:HD12	1:B:278:LEU:HA	1.82	0.45
1:C:253:ASN:O	1:C:256:PRO:HD2	2.16	0.45
1:A:275:LEU:HB3	2:A:281:BOG:H3	1.97	0.45
1:A:128:VAL:O	1:A:132:LEU:HG	2.16	0.45
1:A:208:HIS:HE1	1:A:210:ILE:HB	1.81	0.45
1:C:96:LEU:HD11	1:C:109:LEU:HD11	1.98	0.45
1:A:226:ALA:HA	1:A:227:PRO:HD3	1.86	0.45
1:D:52:THR:HB	4:D:294:HOH:O	2.16	0.45
1:C:102:GLY:O	1:C:103:LYS:HB2	2.17	0.45
1:D:162:GLN:HG3	1:E:134:THR:O	2.17	0.45
1:D:169:MET:HB3	1:D:206:PHE:CE2	2.52	0.45
1:D:96:LEU:O	1:D:97:VAL:HG22	2.17	0.45
1:B:274:TRP:HA	1:B:274:TRP:HE3	1.80	0.45
1:B:190:LYS:HZ2	2:B:285:BOG:C3'	2.30	0.45
1:E:276:ILE:O	1:E:276:ILE:HG22	2.16	0.45
1:D:105:SER:HB3	1:D:107:LYS:N	2.32	0.44
1:B:24:GLY:O	1:B:28:LYS:HG3	2.18	0.44
1:B:106:TRP:C	1:B:108:GLU:H	2.20	0.44
1:C:255:ILE:HB	1:C:256:PRO:CD	2.43	0.44
1:C:248:ASN:O	1:C:252:ASN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:CG1	1:A:105:SER:HA	2.45	0.44
1:A:101:SER:CB	1:A:102:GLY:HA2	2.43	0.44
1:B:98:ALA:HB3	1:B:102:GLY:H	1.82	0.44
1:B:132:LEU:HD13	1:B:225:PHE:CD2	2.52	0.44
1:C:208:HIS:CE1	1:C:210:ILE:HB	2.52	0.44
1:C:274:TRP:HA	1:C:274:TRP:CE3	2.52	0.44
1:C:201:PHE:CD1	1:C:201:PHE:C	2.90	0.44
1:A:109:LEU:HD23	1:A:109:LEU:C	2.37	0.44
1:D:93:VAL:HG23	1:D:116:VAL:CG2	2.40	0.44
1:B:190:LYS:NZ	2:B:285:BOG:H1	2.33	0.44
1:D:25:LYS:NZ	1:D:25:LYS:HB2	2.33	0.44
1:B:103:LYS:C	1:B:105:SER:H	2.20	0.44
1:E:196:LEU:N	1:E:197:PRO:CD	2.81	0.44
1:E:160:PHE:CD2	1:E:256:PRO:HG3	2.53	0.44
1:C:146:LEU:HD11	1:C:234:THR:HB	1.99	0.44
1:A:97:VAL:HG22	1:A:269:VAL:CG1	2.47	0.44
1:B:212:ASN:ND2	1:B:253:ASN:HD21	2.05	0.44
1:B:23:GLU:O	1:B:23:GLU:CG	2.65	0.44
1:A:135:ARG:HD3	4:A:302:HOH:O	2.18	0.44
1:D:27:LYS:HG3	1:D:31:TYR:CE2	2.53	0.43
1:B:160:PHE:HE1	2:B:281:BOG:H7'2	1.83	0.43
1:C:162:GLN:HG3	1:D:134:THR:O	2.17	0.43
1:A:97:VAL:HB	1:A:98:ALA:HB2	2.00	0.43
1:D:161:LEU:H	3:D:285:FMT:C	2.30	0.43
1:C:59:HIS:H	1:C:59:HIS:CD2	2.36	0.43
1:E:146:LEU:HD11	1:E:234:THR:HB	2.00	0.43
1:D:178:VAL:O	1:D:181:THR:OG1	2.33	0.43
1:D:192:MET:SD	2:D:281:BOG:O4	2.71	0.43
1:D:170:CYS:HB2	1:D:206:PHE:HB3	2.00	0.43
1:E:201:PHE:CD1	1:E:201:PHE:C	2.92	0.43
1:E:209:CYS:SG	1:E:261:ASN:ND2	2.89	0.43
1:C:170:CYS:O	1:C:174:VAL:HG23	2.18	0.43
1:D:74:PHE:CG	1:D:202:VAL:HG21	2.54	0.43
1:D:88:LEU:O	1:D:89:PHE:C	2.56	0.43
1:B:120:ASN:HB3	1:B:210:ILE:HG23	2.01	0.43
1:C:99:LYS:O	1:C:100:ALA:HB3	2.19	0.43
1:D:213:MET:O	1:D:217:PRO:HG2	2.19	0.43
1:C:120:ASN:HB3	1:C:210:ILE:HG23	2.01	0.42
1:B:179:TRP:CH2	1:B:272:TRP:CE2	3.08	0.42
1:D:212:ASN:ND2	1:D:253:ASN:HD21	2.05	0.42
1:A:268:PHE:CD1	1:A:268:PHE:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LEU:HD21	2:E:281:BOG:C7'	2.50	0.42
1:A:213:MET:O	1:A:217:PRO:HG2	2.19	0.42
1:A:107:LYS:O	1:A:111:ARG:HB2	2.19	0.42
1:D:105:SER:HB2	1:D:108:GLU:HG2	2.01	0.42
1:B:190:LYS:NZ	2:B:285:BOG:C5	2.74	0.42
1:B:179:TRP:CH2	1:B:272:TRP:CZ2	3.07	0.42
1:C:208:HIS:HE1	1:C:210:ILE:HB	1.85	0.42
1:C:135:ARG:NH2	1:C:227:PRO:HG3	2.35	0.42
1:B:190:LYS:HE3	2:B:285:BOG:H5	2.00	0.42
1:E:141:GLY:HA2	1:E:233:MET:HE1	2.00	0.42
1:A:101:SER:H	1:A:102:GLY:HA2	1.84	0.42
1:A:97:VAL:CG2	1:A:269:VAL:HG22	2.49	0.42
1:A:97:VAL:CB	1:A:98:ALA:HB3	2.50	0.42
1:B:247:VAL:HG13	2:B:283:BOG:H1'1	1.99	0.42
1:A:104:ILE:CB	1:A:105:SER:HA	2.49	0.42
1:E:135:ARG:HH22	1:E:227:PRO:HG3	1.84	0.42
1:B:104:ILE:HD12	1:B:108:GLU:HG2	2.02	0.42
1:D:94:LEU:HB3	1:D:97:VAL:CG1	2.46	0.42
1:B:186:SER:HA	2:B:285:BOG:O2	2.20	0.42
1:A:102:GLY:HA3	1:A:103:LYS:HA	1.90	0.42
1:A:130:ILE:O	1:A:134:THR:HG23	2.20	0.42
1:E:233:MET:HB3	1:E:233:MET:HE2	1.93	0.41
1:C:92:SER:O	1:C:94:LEU:N	2.52	0.41
1:A:95:ILE:HA	1:A:95:ILE:HD12	1.94	0.41
1:A:27:LYS:HG2	1:A:31:TYR:HE2	1.85	0.41
1:D:89:PHE:CD2	1:D:117:TYR:HD1	2.37	0.41
1:E:213:MET:O	1:E:217:PRO:HG2	2.20	0.41
1:D:216:VAL:HB	1:D:217:PRO:HD3	2.01	0.41
1:B:248:ASN:O	1:B:252:ASN:HB2	2.19	0.41
1:D:103:LYS:HB3	1:D:104:ILE:CA	2.38	0.41
2:E:310:BOG:H1'1	2:E:310:BOG:H6'1	2.02	0.41
1:B:94:LEU:HD13	1:B:94:LEU:H	1.85	0.41
1:A:179:TRP:HH2	2:A:281:BOG:O6	2.03	0.41
1:D:25:LYS:HG3	1:D:27:LYS:HB2	2.02	0.41
1:E:188:THR:O	1:E:192:MET:HG2	2.20	0.41
1:B:216:VAL:HB	1:B:217:PRO:HD3	2.02	0.41
1:B:104:ILE:O	1:B:104:ILE:HG22	2.21	0.41
1:C:213:MET:O	1:C:217:PRO:HG2	2.20	0.41
1:C:102:GLY:C	1:C:104:ILE:H	2.24	0.41
1:C:96:LEU:HD12	1:C:97:VAL:HG13	2.03	0.41
1:E:144:LEU:C	1:E:144:LEU:HD23	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HB3	1:E:271:MET:HE3	2.03	0.41
1:D:106:TRP:CZ3	1:D:109:LEU:HD23	2.56	0.41
1:C:135:ARG:HH22	1:C:227:PRO:HG3	1.86	0.41
1:C:160:PHE:CD2	1:C:256:PRO:HG3	2.56	0.41
1:B:90:THR:HG21	1:B:208:HIS:CE1	2.55	0.41
1:C:210:ILE:O	1:C:213:MET:HB2	2.20	0.41
1:C:103:LYS:HE2	1:C:103:LYS:HB3	1.87	0.41
1:E:74:PHE:CG	1:E:202:VAL:HG21	2.55	0.41
1:A:89:PHE:N	1:A:120:ASN:HD21	2.07	0.40
1:B:209:CYS:N	1:B:261:ASN:HD21	2.06	0.40
1:D:107:LYS:O	1:D:107:LYS:HD2	2.21	0.40
1:B:243:ASP:CA	2:B:286:BOG:H4	2.51	0.40
1:A:179:TRP:NE1	1:B:84:THR:HG22	2.36	0.40
1:A:185:ARG:NH1	1:E:185:ARG:NH1	2.68	0.40
1:D:121:LEU:HD12	1:D:121:LEU:HA	1.87	0.40
1:B:162:GLN:HG3	1:C:134:THR:O	2.21	0.40
1:A:99:LYS:O	1:A:99:LYS:HG2	2.22	0.40
1:A:201:PHE:C	1:A:201:PHE:CD1	2.93	0.40
1:A:168:LEU:HD22	1:A:264:GLY:CA	2.52	0.40
1:D:26:ALA:HB1	4:D:313:HOH:O	2.20	0.40
1:B:82:VAL:O	2:B:285:BOG:H5'2	2.22	0.40
1:D:279:LYS:HB2	1:D:279:LYS:HZ3	1.87	0.40
1:B:96:LEU:HB3	1:B:97:VAL:H	1.66	0.40
1:C:105:SER:O	1:C:106:TRP:HB2	2.21	0.40
3:C:287:FMT:H	4:C:324:HOH:O	2.21	0.40
1:D:244:LEU:HD12	1:D:244:LEU:HA	1.90	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	256/280 (91%)	245 (96%)	9 (4%)	2 (1%)	24 41
1	B	254/280 (91%)	239 (94%)	9 (4%)	6 (2%)	7 11
1	C	253/280 (90%)	240 (95%)	10 (4%)	3 (1%)	16 29
1	D	253/280 (90%)	242 (96%)	8 (3%)	3 (1%)	16 29
1	E	255/280 (91%)	248 (97%)	6 (2%)	1 (0%)	39 61
All	All	1271/1400 (91%)	1214 (96%)	42 (3%)	15 (1%)	16 29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	ILE
1	C	95	ILE
1	C	97	VAL
1	D	97	VAL
1	B	24	GLY
1	B	100	ALA
1	C	93	VAL
1	D	89	PHE
1	A	107	LYS
1	B	93	VAL
1	B	105	SER
1	D	96	LEU
1	E	89	PHE
1	A	104	ILE
1	B	98	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	207/226 (92%)	192 (93%)	15 (7%)	18 33
1	B	206/226 (91%)	191 (93%)	15 (7%)	17 32
1	C	206/226 (91%)	197 (96%)	9 (4%)	35 60
1	D	206/226 (91%)	192 (93%)	14 (7%)	20 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	207/226 (92%)	195 (94%)	12 (6%)	25 45
All	All	1032/1130 (91%)	967 (94%)	65 (6%)	22 40

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	50	PHE
1	A	60	ASP
1	A	91	SER
1	A	96	LEU
1	A	103	LYS
1	A	104	ILE
1	A	107	LYS
1	A	111	ARG
1	A	179	TRP
1	A	185	ARG
1	A	201	PHE
1	A	244	LEU
1	A	254	LEU
1	A	275	LEU
1	B	25	LYS
1	B	48	PHE
1	B	50	PHE
1	B	94	LEU
1	B	96	LEU
1	B	108	GLU
1	B	201	PHE
1	B	204	SER
1	B	244	LEU
1	B	247	VAL
1	B	254	LEU
1	B	267	VAL
1	B	274	TRP
1	B	275	LEU
1	B	278	LEU
1	C	48	PHE
1	C	50	PHE
1	C	96	LEU
1	C	104	ILE
1	C	113	TRP
1	C	201	PHE

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Mol	Chain	Res	Type
1	C	204	SER
1	C	254	LEU
1	C	279	LYS
1	D	25	LYS
1	D	48	PHE
1	D	50	PHE
1	D	93	VAL
1	D	106	TRP
1	D	107	LYS
1	D	171	ASN
1	D	185	ARG
1	D	201	PHE
1	D	204	SER
1	D	228	GLU
1	D	244	LEU
1	D	254	LEU
1	D	279	LYS
1	E	25	LYS
1	E	48	PHE
1	E	50	PHE
1	E	94	LEU
1	E	96	LEU
1	E	99	LYS
1	E	171	ASN
1	E	201	PHE
1	E	244	LEU
1	E	254	LEU
1	E	273	TYR
1	E	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	136	GLN
1	A	253	ASN
1	A	261	ASN
1	B	120	ASN
1	B	136	GLN
1	B	253	ASN
1	B	261	ASN
1	C	120	ASN

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Mol	Chain	Res	Type
1	C	136	GLN
1	C	253	ASN
1	C	261	ASN
1	D	112	ASN
1	D	120	ASN
1	D	136	GLN
1	D	171	ASN
1	D	253	ASN
1	D	261	ASN
1	E	112	ASN
1	E	120	ASN
1	E	136	GLN
1	E	171	ASN
1	E	253	ASN
1	E	261	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

53 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	BOG	A	281	-	20,20,20	1.95	2 (10%)	25,25,25	3.29	13 (52%)
2	BOG	A	282	-	20,20,20	0.99	1 (5%)	25,25,25	3.09	13 (52%)
2	BOG	A	283	-	20,20,20	0.85	1 (5%)	25,25,25	2.68	10 (40%)
3	FMT	A	284	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	285	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	286	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	287	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	288	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	289	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	290	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	291	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	292	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BOG	B	281	-	20,20,20	0.89	0	25,25,25	3.23	13 (52%)
2	BOG	B	282	-	20,20,20	0.88	0	25,25,25	3.28	14 (56%)
2	BOG	B	283	-	20,20,20	0.90	0	25,25,25	3.35	12 (48%)
2	BOG	B	284	-	20,20,20	0.84	0	25,25,25	3.43	12 (48%)
2	BOG	B	285	-	20,20,20	0.90	0	25,25,25	2.90	11 (44%)
2	BOG	B	286	-	20,20,20	0.85	0	25,25,25	3.14	12 (48%)
3	FMT	B	287	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	288	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	289	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	290	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	291	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	292	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	293	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	294	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	295	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BOG	C	281	-	20,20,20	0.84	0	25,25,25	3.10	14 (56%)
2	BOG	C	282	-	20,20,20	0.84	0	25,25,25	3.04	15 (60%)
3	FMT	C	283	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	284	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	285	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	286	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	287	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	288	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BOG	D	281	-	20,20,20	0.86	1 (5%)	25,25,25	3.23	11 (44%)
3	FMT	D	282	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	283	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	284	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	285	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FMT	D	286	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	287	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	288	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BOG	E	281	-	20,20,20	0.89	0	25,25,25	3.17	13 (52%)
3	FMT	E	282	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	283	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	284	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	285	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	286	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	287	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BOG	E	310	-	20,20,20	0.88	1 (5%)	25,25,25	2.77	12 (48%)
3	FMT	E	311	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	312	-	0,2,2	0.00	-	0,1,1	0.00	-

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	BOG	A	281	-	-	0/11/31/31	0/1/1/1
2	BOG	A	282	-	1/1/5/5	0/11/31/31	0/1/1/1
2	BOG	A	283	-	-	0/11/31/31	0/1/1/1
3	FMT	A	284	-	-	0/0/0/0	0/0/0/0
3	FMT	A	285	-	-	0/0/0/0	0/0/0/0
3	FMT	A	286	-	-	0/0/0/0	0/0/0/0
3	FMT	A	287	-	-	0/0/0/0	0/0/0/0
3	FMT	A	288	-	-	0/0/0/0	0/0/0/0
3	FMT	A	289	-	-	0/0/0/0	0/0/0/0
3	FMT	A	290	-	-	0/0/0/0	0/0/0/0
3	FMT	A	291	-	-	0/0/0/0	0/0/0/0
3	FMT	A	292	-	-	0/0/0/0	0/0/0/0
2	BOG	B	281	-	-	0/11/31/31	0/1/1/1
2	BOG	B	282	-	-	0/11/31/31	0/1/1/1
2	BOG	B	283	-	-	0/11/31/31	0/1/1/1
2	BOG	B	284	-	-	0/11/31/31	0/1/1/1
2	BOG	B	285	-	-	0/11/31/31	0/1/1/1
2	BOG	B	286	-	-	0/11/31/31	0/1/1/1
3	FMT	B	287	-	-	0/0/0/0	0/0/0/0
3	FMT	B	288	-	-	0/0/0/0	0/0/0/0
3	FMT	B	289	-	-	0/0/0/0	0/0/0/0
3	FMT	B	290	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMT	B	291	-	-	0/0/0/0	0/0/0/0
3	FMT	B	292	-	-	0/0/0/0	0/0/0/0
3	FMT	B	293	-	-	0/0/0/0	0/0/0/0
3	FMT	B	294	-	-	0/0/0/0	0/0/0/0
3	FMT	B	295	-	-	0/0/0/0	0/0/0/0
2	BOG	C	281	-	-	0/11/31/31	0/1/1/1
2	BOG	C	282	-	-	0/11/31/31	0/1/1/1
3	FMT	C	283	-	-	0/0/0/0	0/0/0/0
3	FMT	C	284	-	-	0/0/0/0	0/0/0/0
3	FMT	C	285	-	-	0/0/0/0	0/0/0/0
3	FMT	C	286	-	-	0/0/0/0	0/0/0/0
3	FMT	C	287	-	-	0/0/0/0	0/0/0/0
3	FMT	C	288	-	-	0/0/0/0	0/0/0/0
2	BOG	D	281	-	-	0/11/31/31	0/1/1/1
3	FMT	D	282	-	-	0/0/0/0	0/0/0/0
3	FMT	D	283	-	-	0/0/0/0	0/0/0/0
3	FMT	D	284	-	-	0/0/0/0	0/0/0/0
3	FMT	D	285	-	-	0/0/0/0	0/0/0/0
3	FMT	D	286	-	-	0/0/0/0	0/0/0/0
3	FMT	D	287	-	-	0/0/0/0	0/0/0/0
3	FMT	D	288	-	-	0/0/0/0	0/0/0/0
2	BOG	E	281	-	-	0/11/31/31	0/1/1/1
3	FMT	E	282	-	-	0/0/0/0	0/0/0/0
3	FMT	E	283	-	-	0/0/0/0	0/0/0/0
3	FMT	E	284	-	-	0/0/0/0	0/0/0/0
3	FMT	E	285	-	-	0/0/0/0	0/0/0/0
3	FMT	E	286	-	-	0/0/0/0	0/0/0/0
3	FMT	E	287	-	-	0/0/0/0	0/0/0/0
2	BOG	E	310	-	-	0/11/31/31	0/1/1/1
3	FMT	E	311	-	-	0/0/0/0	0/0/0/0
3	FMT	E	312	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	281	BOG	O5-C1	-4.37	1.30	1.41
2	A	282	BOG	O2-C2	-3.00	1.35	1.43
2	E	310	BOG	O2-C2	-2.13	1.37	1.43
2	A	283	BOG	O2-C2	-2.07	1.38	1.43
2	D	281	BOG	O2-C2	-2.03	1.38	1.43
2	A	281	BOG	O5-C5	6.57	1.60	1.44

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	282	BOG	C1-O5-C5	-3.23	107.48	113.75
2	A	281	BOG	O5-C1-O1	-2.84	103.21	110.05
2	A	281	BOG	C4-C3-C2	-2.84	105.49	110.79
2	A	282	BOG	C4-C3-C2	-2.61	105.93	110.79
2	C	281	BOG	C1-O5-C5	-2.50	108.89	113.75
2	C	282	BOG	C1-O5-C5	-2.35	109.19	113.75
2	D	281	BOG	C1-O5-C5	-2.24	109.39	113.75
2	A	282	BOG	C1-O5-C5	-2.18	109.52	113.75
2	B	286	BOG	C1-O5-C5	-2.12	109.62	113.75
2	B	281	BOG	C1-O5-C5	-2.02	109.82	113.75
2	B	282	BOG	O1-C1'-C2'	2.04	117.99	109.88
2	E	281	BOG	O6-C6-C5	2.05	118.12	111.33
2	A	282	BOG	C3-C4-C5	2.07	113.80	110.20
2	E	310	BOG	O5-C5-C4	2.08	113.59	109.68
2	C	282	BOG	C6-C5-C4	2.10	118.20	113.02
2	B	281	BOG	O6-C6-C5	2.14	118.40	111.33
2	C	281	BOG	O6-C6-C5	2.15	118.45	111.33
2	B	284	BOG	C6-C5-C4	2.16	118.33	113.02
2	E	281	BOG	O1-C1'-C2'	2.18	118.53	109.88
2	B	285	BOG	O1-C1'-C2'	2.23	118.74	109.88
2	C	281	BOG	O1-C1'-C2'	2.23	118.77	109.88
2	B	284	BOG	O6-C6-C5	2.27	118.85	111.33
2	B	281	BOG	C6-C5-C4	2.36	118.84	113.02
2	A	281	BOG	O1-C1'-C2'	2.39	119.39	109.88
2	B	283	BOG	O1-C1'-C2'	2.44	119.57	109.88
2	E	281	BOG	C6-C5-C4	2.45	119.07	113.02
2	C	282	BOG	O6-C6-C5	2.48	119.54	111.33
2	B	285	BOG	O4-C4-C5	2.50	115.87	109.24
2	B	286	BOG	C6-C5-C4	2.51	119.22	113.02
2	C	282	BOG	C4-C3-C2	2.68	115.79	110.79
2	B	283	BOG	O6-C6-C5	2.70	120.26	111.33
2	C	281	BOG	C6-C5-C4	2.71	119.70	113.02
2	A	282	BOG	C6-C5-C4	2.72	119.73	113.02
2	C	282	BOG	O3-C3-C2	2.72	116.47	110.34
2	C	282	BOG	O4-C4-C3	2.72	116.47	110.34
2	C	282	BOG	O4-C4-C5	2.78	116.60	109.24
2	A	281	BOG	C1-O5-C5	2.79	119.15	113.75
2	C	282	BOG	C1'-O1-C1	2.80	118.84	113.94
2	B	285	BOG	O3-C3-C2	2.82	116.68	110.34
2	E	310	BOG	C3-C4-C5	2.84	115.15	110.20
2	A	283	BOG	O5-C1-O1	2.87	116.97	110.05
2	E	310	BOG	O4-C4-C5	2.92	116.97	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	282	BOG	O3-C3-C4	2.93	116.93	110.34
2	B	282	BOG	C6-C5-C4	2.93	120.25	113.02
2	B	282	BOG	O2-C2-C3	2.94	116.94	110.34
2	E	310	BOG	O3-C3-C4	2.98	117.06	110.34
2	B	283	BOG	C1'-O1-C1	3.06	119.28	113.94
2	A	283	BOG	O4-C4-C3	3.07	117.25	110.34
2	A	282	BOG	C1'-O1-C1	3.10	119.36	113.94
2	B	284	BOG	O3-C3-C4	3.12	117.35	110.34
2	A	282	BOG	O2-C2-C3	3.12	117.35	110.34
2	A	283	BOG	O2-C2-C3	3.14	117.41	110.34
2	B	282	BOG	O2-C2-C1	3.16	116.95	110.02
2	A	283	BOG	O3-C3-C4	3.16	117.46	110.34
2	E	310	BOG	O4-C4-C3	3.18	117.50	110.34
2	E	310	BOG	O3-C3-C2	3.21	117.56	110.34
2	C	281	BOG	O3-C3-C2	3.23	117.62	110.34
2	C	282	BOG	O3-C3-C4	3.28	117.73	110.34
2	A	282	BOG	O5-C1-O1	3.30	118.00	110.05
2	E	310	BOG	O5-C1-O1	3.35	118.12	110.05
2	B	281	BOG	O4-C4-C3	3.40	117.99	110.34
2	B	284	BOG	O4-C4-C3	3.41	118.02	110.34
2	A	281	BOG	C1'-O1-C1	3.41	119.91	113.94
2	A	283	BOG	O2-C2-C1	3.45	117.59	110.02
2	D	281	BOG	O4-C4-C5	3.46	118.40	109.24
2	B	284	BOG	O5-C1-O1	3.46	118.40	110.05
2	E	281	BOG	O2-C2-C3	3.47	118.15	110.34
2	E	281	BOG	O5-C1-O1	3.48	118.43	110.05
2	B	286	BOG	C1'-O1-C1	3.48	120.03	113.94
2	C	281	BOG	O2-C2-C3	3.49	118.20	110.34
2	E	310	BOG	C1'-O1-C1	3.50	120.06	113.94
2	A	283	BOG	O5-C5-C6	3.52	115.25	106.36
2	B	283	BOG	O4-C4-C5	3.52	118.58	109.24
2	B	284	BOG	O4-C4-C5	3.53	118.60	109.24
2	B	285	BOG	O3-C3-C4	3.55	118.32	110.34
2	E	310	BOG	O2-C2-C3	3.55	118.34	110.34
2	E	281	BOG	O3-C3-C2	3.57	118.39	110.34
2	D	281	BOG	O2-C2-C3	3.61	118.47	110.34
2	C	281	BOG	O4-C4-C3	3.61	118.47	110.34
2	C	281	BOG	O3-C3-C4	3.62	118.48	110.34
2	B	282	BOG	C1-C2-C3	3.62	117.10	109.97
2	B	281	BOG	O4-C4-C5	3.65	118.91	109.24
2	C	281	BOG	O4-C4-C5	3.65	118.91	109.24
2	B	281	BOG	O2-C2-C3	3.68	118.62	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	281	BOG	C1'-O1-C1	3.69	120.38	113.94
2	C	282	BOG	O2-C2-C3	3.69	118.64	110.34
2	B	285	BOG	O2-C2-C1	3.72	118.17	110.02
2	A	283	BOG	O4-C4-C5	3.74	119.15	109.24
2	B	285	BOG	O2-C2-C3	3.74	118.77	110.34
2	E	310	BOG	O2-C2-C1	3.75	118.25	110.02
2	D	281	BOG	O5-C1-O1	3.76	119.12	110.05
2	B	283	BOG	O2-C2-C3	3.77	118.82	110.34
2	B	281	BOG	O3-C3-C2	3.77	118.84	110.34
2	B	281	BOG	O5-C1-O1	3.78	119.17	110.05
2	B	286	BOG	O4-C4-C5	3.80	119.30	109.24
2	E	281	BOG	O4-C4-C5	3.82	119.38	109.24
2	A	281	BOG	O4-C4-C5	3.85	119.43	109.24
2	B	286	BOG	O5-C1-O1	3.85	119.33	110.05
2	A	283	BOG	C1'-O1-C1	3.89	120.74	113.94
2	B	284	BOG	O3-C3-C2	3.90	119.11	110.34
2	B	281	BOG	O3-C3-C4	3.92	119.15	110.34
2	B	282	BOG	O4-C4-C5	3.93	119.64	109.24
2	B	282	BOG	O3-C3-C2	3.93	119.19	110.34
2	B	283	BOG	O4-C4-C3	3.94	119.20	110.34
2	B	286	BOG	O3-C3-C2	3.95	119.22	110.34
2	B	285	BOG	C1'-O1-C1	3.95	120.85	113.94
2	B	286	BOG	O3-C3-C4	3.95	119.24	110.34
2	B	283	BOG	O3-C3-C2	3.97	119.26	110.34
2	B	286	BOG	O4-C4-C3	3.97	119.27	110.34
2	B	286	BOG	O2-C2-C3	4.00	119.33	110.34
2	C	281	BOG	C1'-O1-C1	4.00	120.93	113.94
2	D	281	BOG	C1'-O1-C1	4.00	120.94	113.94
2	B	285	BOG	O4-C4-C3	4.02	119.40	110.34
2	C	281	BOG	O5-C1-O1	4.02	119.74	110.05
2	B	282	BOG	O4-C4-C3	4.03	119.41	110.34
2	D	281	BOG	O3-C3-C2	4.03	119.41	110.34
2	B	282	BOG	O3-C3-C4	4.04	119.43	110.34
2	C	282	BOG	O5-C1-O1	4.04	119.79	110.05
2	B	282	BOG	O5-C1-O1	4.05	119.81	110.05
2	A	281	BOG	O4-C4-C3	4.05	119.47	110.34
2	D	281	BOG	O3-C3-C4	4.06	119.48	110.34
2	C	281	BOG	O2-C2-C1	4.07	118.95	110.02
2	A	282	BOG	O5-C5-C6	4.08	116.68	106.36
2	C	282	BOG	O2-C2-C1	4.11	119.02	110.02
2	E	310	BOG	O5-C5-C6	4.14	116.81	106.36
2	B	282	BOG	C1'-O1-C1	4.19	121.26	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	281	BOG	O2-C2-C3	4.20	119.79	110.34
2	B	283	BOG	O5-C1-O1	4.21	120.19	110.05
2	D	281	BOG	O2-C2-C1	4.21	119.26	110.02
2	E	281	BOG	O4-C4-C3	4.23	119.87	110.34
2	A	281	BOG	O3-C3-C4	4.25	119.90	110.34
2	C	282	BOG	C3-C4-C5	4.25	117.61	110.20
2	B	286	BOG	O2-C2-C1	4.26	119.35	110.02
2	E	281	BOG	O3-C3-C4	4.28	119.97	110.34
2	A	283	BOG	O3-C3-C2	4.31	120.05	110.34
2	B	283	BOG	O3-C3-C4	4.37	120.17	110.34
2	A	281	BOG	O5-C5-C4	4.37	117.88	109.68
2	B	281	BOG	C1'-O1-C1	4.41	121.64	113.94
2	D	281	BOG	O4-C4-C3	4.41	120.26	110.34
2	B	284	BOG	O2-C2-C3	4.44	120.33	110.34
2	A	281	BOG	O3-C3-C2	4.52	120.52	110.34
2	C	282	BOG	O5-C5-C6	4.58	117.92	106.36
2	B	281	BOG	O2-C2-C1	4.61	120.12	110.02
2	E	281	BOG	O2-C2-C1	4.70	120.33	110.02
2	B	281	BOG	O5-C5-C6	4.77	118.42	106.36
2	A	281	BOG	O2-C2-C1	4.87	120.69	110.02
2	B	284	BOG	O5-C5-C6	4.92	118.78	106.36
2	B	284	BOG	O2-C2-C1	4.98	120.93	110.02
2	B	286	BOG	O5-C5-C6	5.08	119.19	106.36
2	A	282	BOG	O4-C4-C5	5.08	122.70	109.24
2	E	281	BOG	O5-C5-C6	5.10	119.23	106.36
2	B	283	BOG	O2-C2-C1	5.12	121.25	110.02
2	B	284	BOG	C1'-O1-C1	5.15	122.94	113.94
2	B	285	BOG	O5-C1-O1	5.18	122.53	110.05
2	B	283	BOG	O5-C5-C6	5.20	119.51	106.36
2	C	281	BOG	O5-C5-C6	5.25	119.62	106.36
2	A	282	BOG	O4-C4-C3	5.42	122.54	110.34
2	D	281	BOG	O5-C5-C6	5.59	120.48	106.36
2	A	282	BOG	O3-C3-C2	5.66	123.07	110.34
2	B	282	BOG	O5-C5-C6	5.81	121.03	106.36
2	B	285	BOG	O5-C5-C6	6.26	122.19	106.36
2	B	285	BOG	O1-C1-C2	6.39	116.11	108.04
2	A	283	BOG	O1-C1-C2	7.36	117.33	108.04
2	A	282	BOG	O1-C1-C2	7.60	117.64	108.04
2	E	310	BOG	O1-C1-C2	7.78	117.87	108.04
2	B	282	BOG	O1-C1-C2	8.40	118.65	108.04
2	C	282	BOG	O1-C1-C2	8.42	118.67	108.04
2	C	281	BOG	O1-C1-C2	8.60	118.90	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	286	BOG	O1-C1-C2	8.78	119.13	108.04
2	E	281	BOG	O1-C1-C2	8.95	119.35	108.04
2	D	281	BOG	O1-C1-C2	9.08	119.51	108.04
2	A	281	BOG	O1-C1-C2	9.16	119.60	108.04
2	B	281	BOG	O1-C1-C2	9.63	120.20	108.04
2	B	283	BOG	O1-C1-C2	9.71	120.30	108.04
2	B	284	BOG	O1-C1-C2	10.59	121.42	108.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	282	BOG	C4

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	281	BOG	3	0
2	A	282	BOG	8	0
3	A	285	FMT	2	0
3	A	292	FMT	1	0
2	B	281	BOG	1	0
2	B	282	BOG	2	0
2	B	283	BOG	16	0
2	B	285	BOG	17	0
2	B	286	BOG	3	0
3	B	287	FMT	1	0
3	B	290	FMT	2	0
3	B	292	FMT	1	0
2	C	281	BOG	3	0
2	C	282	BOG	1	0
3	C	283	FMT	2	0
3	C	287	FMT	1	0
2	D	281	BOG	4	0
3	D	282	FMT	1	0
3	D	285	FMT	1	0
2	E	281	BOG	3	0
2	E	310	BOG	4	0
3	E	311	FMT	1	0
3	E	312	FMT	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	258/280 (92%)	0.14	25 (9%)	10 10	23, 37, 119, 178	0
1	B	256/280 (91%)	0.21	30 (11%)	6 6	22, 35, 148, 204	0
1	C	255/280 (91%)	0.35	33 (12%)	5 4	23, 39, 152, 238	0
1	D	255/280 (91%)	0.48	38 (14%)	3 3	31, 50, 163, 210	0
1	E	257/280 (91%)	0.31	32 (12%)	5 5	26, 45, 111, 162	0
All	All	1281/1400 (91%)	0.30	158 (12%)	5 5	22, 41, 138, 238	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	ALA	9.5
1	C	98	ALA	8.6
1	D	98	ALA	8.1
1	C	97	VAL	7.4
1	C	103	LYS	7.0
1	E	97	VAL	6.8
1	B	95	ILE	6.4
1	B	96	LEU	6.0
1	C	102	GLY	6.0
1	C	105	SER	6.0
1	D	104	ILE	5.8
1	C	99	LYS	5.8
1	D	105	SER	5.8
1	E	106	TRP	5.7
1	A	104	ILE	5.7
1	D	106	TRP	5.6
1	D	101	SER	5.6
1	D	95	ILE	5.6
1	C	31	TYR	5.5
1	B	102	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	5.4
1	A	31	TYR	5.3
1	C	96	LEU	5.3
1	D	97	VAL	5.2
1	C	100	ALA	5.2
1	B	104	ILE	5.2
1	B	105	SER	4.9
1	A	28	LYS	4.7
1	B	97	VAL	4.5
1	E	100	ALA	4.4
1	E	98	ALA	4.3
1	E	278	LEU	4.3
1	C	101	SER	4.2
1	D	31	TYR	4.2
1	E	231	TRP	4.1
1	E	94	LEU	4.1
1	C	94	LEU	4.1
1	B	99	LYS	4.1
1	E	96	LEU	4.1
1	A	99	LYS	4.0
1	A	26	ALA	4.0
1	B	272	TRP	4.0
1	E	95	ILE	4.0
1	D	96	LEU	4.0
1	D	103	LYS	4.0
1	A	109	LEU	3.9
1	D	92	SER	3.9
1	D	108	GLU	3.8
1	A	106	TRP	3.7
1	D	272	TRP	3.6
1	A	105	SER	3.6
1	A	22	GLY	3.6
1	C	104	ILE	3.6
1	B	23	GLU	3.6
1	B	106	TRP	3.6
1	C	272	TRP	3.6
1	D	93	VAL	3.5
1	B	94	LEU	3.5
1	D	195	ILE	3.4
1	E	228	GLU	3.4
1	E	103	LYS	3.4
1	C	29	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	196	LEU	3.3
1	C	27	LYS	3.2
1	B	275	LEU	3.2
1	C	30	ALA	3.1
1	E	232	ALA	3.1
1	E	277	TYR	3.1
1	C	277	TYR	3.1
1	D	26	ALA	3.1
1	C	276	ILE	3.0
1	D	109	LEU	3.0
1	C	72	LEU	3.0
1	D	69	LEU	3.0
1	C	107	LYS	3.0
1	C	95	ILE	3.0
1	C	195	ILE	2.9
1	E	237	ASN	2.9
1	A	103	LYS	2.9
1	A	23	GLU	2.9
1	E	92	SER	2.9
1	D	276	ILE	2.9
1	D	278	LEU	2.9
1	B	277	TYR	2.8
1	B	274	TRP	2.8
1	A	27	LYS	2.8
1	D	275	LEU	2.7
1	D	90	THR	2.7
1	E	99	LYS	2.7
1	B	26	ALA	2.7
1	A	60	ASP	2.7
1	D	28	LYS	2.7
1	B	278	LEU	2.7
1	C	109	LEU	2.7
1	C	25	LYS	2.7
1	E	26	ALA	2.7
1	C	69	LEU	2.6
1	C	192	MET	2.6
1	C	28	LYS	2.6
1	E	230	PHE	2.6
1	E	102	GLY	2.6
1	D	94	LEU	2.6
1	E	195	ILE	2.6
1	A	102	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	277	TYR	2.5
1	B	101	SER	2.5
1	B	31	TYR	2.5
1	D	274	TRP	2.5
1	A	192	MET	2.5
1	D	192	MET	2.5
1	C	196	LEU	2.5
1	C	225	PHE	2.4
1	E	101	SER	2.4
1	A	59	HIS	2.4
1	A	191	VAL	2.4
1	B	109	LEU	2.4
1	E	108	GLU	2.4
1	C	106	TRP	2.4
1	A	277	TYR	2.4
1	B	195	ILE	2.4
1	D	27	LYS	2.3
1	B	69	LEU	2.3
1	E	236	ALA	2.3
1	E	107	LYS	2.3
1	D	73	ALA	2.3
1	A	29	ALA	2.2
1	D	273	TYR	2.2
1	A	96	LEU	2.2
1	B	72	LEU	2.2
1	E	275	LEU	2.2
1	D	72	LEU	2.2
1	D	107	LYS	2.2
1	B	92	SER	2.2
1	E	276	ILE	2.2
1	A	24	GLY	2.2
1	D	259	LEU	2.2
1	B	103	LYS	2.2
1	D	114	THR	2.2
1	B	59	HIS	2.2
1	E	73	ALA	2.2
1	D	237	ASN	2.2
1	B	77	GLY	2.1
1	A	94	LEU	2.1
1	D	247	VAL	2.1
1	C	228	GLU	2.1
1	E	273	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	76	LEU	2.1
1	E	72	LEU	2.1
1	A	101	SER	2.1
1	C	173	LEU	2.1
1	E	235	GLY	2.0
1	B	108	GLU	2.0
1	B	73	ALA	2.0
1	A	196	LEU	2.0
1	E	27	LYS	2.0
1	A	100	ALA	2.0
1	E	91	SER	2.0
1	C	118	PHE	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
2	BOG	B	286	20/20	0.70	0.52	48.59	57,87,105,106	0
3	FMT	C	283	3/3	0.82	0.23	19.26	64,64,66,69	0
3	FMT	B	292	3/3	0.84	0.22	16.16	96,96,97,97	0
3	FMT	B	287	3/3	0.82	0.39	12.44	76,76,82,83	0
2	BOG	A	282	20/20	0.77	0.54	12.05	67,104,121,126	0
2	BOG	E	281	20/20	0.79	0.64	11.28	70,109,129,130	0
2	BOG	B	282	20/20	0.76	0.63	9.93	87,96,124,124	0
3	FMT	C	284	3/3	0.87	0.43	9.81	82,82,85,87	0
3	FMT	E	285	3/3	0.77	0.51	9.69	72,72,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FMT	E	283	3/3	0.87	0.23	9.60	51,51,60,63	0
2	BOG	D	281	20/20	0.78	0.69	9.02	83,105,113,114	0
2	BOG	B	283	20/20	0.84	0.26	8.38	28,81,96,96	0
3	FMT	D	288	3/3	0.93	0.24	7.46	78,78,80,81	0
2	BOG	C	281	20/20	0.82	0.55	6.81	72,99,117,122	0
2	BOG	B	281	20/20	0.81	0.36	6.55	59,83,92,96	0
2	BOG	B	284	20/20	0.77	0.25	6.33	33,73,108,109	0
2	BOG	B	285	20/20	0.79	0.33	6.17	41,60,89,90	0
2	BOG	A	281	20/20	0.60	0.37	5.93	55,88,134,134	0
3	FMT	B	294	3/3	0.93	0.30	5.23	65,65,67,68	0
3	FMT	A	286	3/3	0.93	0.24	5.20	46,46,51,58	0
3	FMT	D	283	3/3	0.81	0.39	5.14	71,71,72,73	0
3	FMT	B	288	3/3	0.88	0.41	3.86	55,55,69,76	0
3	FMT	A	292	3/3	0.97	0.24	3.51	59,59,67,71	0
3	FMT	B	295	3/3	0.92	0.21	3.39	60,60,66,67	0
3	FMT	E	286	3/3	0.80	0.31	3.35	68,68,68,72	0
3	FMT	A	284	3/3	0.79	0.37	3.00	98,98,101,103	0
2	BOG	C	282	20/20	0.82	0.30	2.82	55,82,108,109	0
3	FMT	A	285	3/3	0.89	0.41	2.74	59,59,72,77	0
3	FMT	B	291	3/3	0.73	0.22	2.26	69,69,70,72	0
3	FMT	E	311	3/3	0.97	0.24	2.13	61,61,65,70	0
2	BOG	E	310	20/20	0.85	0.28	1.37	53,71,78,79	0
3	FMT	D	284	3/3	0.94	0.20	1.06	58,58,64,65	0
3	FMT	C	287	3/3	0.89	0.15	1.03	55,55,62,69	0
2	BOG	A	283	20/20	0.91	0.18	0.59	55,62,71,73	0
3	FMT	A	291	3/3	0.89	0.13	0.38	67,67,75,77	0
3	FMT	A	288	3/3	0.93	0.18	0.04	70,70,71,72	0
3	FMT	E	287	3/3	0.91	0.14	-0.12	78,78,82,82	0
3	FMT	C	288	3/3	0.97	0.12	-0.30	58,58,66,69	0
3	FMT	D	282	3/3	0.87	0.15	-0.30	92,92,95,96	0
3	FMT	E	312	3/3	0.91	0.13	-0.45	66,66,68,69	0
3	FMT	C	286	3/3	0.89	0.12	-1.39	91,91,94,95	0
3	FMT	D	286	3/3	0.83	0.17	-	76,76,79,80	0
3	FMT	E	282	3/3	0.89	0.26	-	66,66,71,76	0
3	FMT	C	285	3/3	0.94	0.11	-	71,71,72,73	0
3	FMT	B	289	3/3	0.88	0.27	-	72,72,79,85	0
3	FMT	B	293	3/3	0.88	0.25	-	88,88,89,91	0
3	FMT	D	285	3/3	0.87	0.35	-	69,69,70,73	0
3	FMT	D	287	3/3	0.76	0.17	-	80,80,84,84	0
3	FMT	A	287	3/3	0.70	0.86	-	88,88,90,91	0
3	FMT	A	289	3/3	0.89	0.19	-	51,51,70,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FMT	A	290	3/3	0.91	0.18	-	50,50,64,68	0
3	FMT	B	290	3/3	0.91	0.41	-	70,70,77,80	0
3	FMT	E	284	3/3	0.96	0.19	-	80,80,85,87	0

6.5 Other polymers (i)

There are no such residues in this entry.