Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:21 AM GMT

PDB ID	:	2WSB
Title	:	CRYSTAL STRUCTURE OF THE SHORT-CHAIN DEHYDROGENASE GALACTITOL-DEHYDROGENASE (GATDH) OF RHODOBACTER SPHAEROIDES IN COMPLEX WITH NAD
Authors	:	Carius, Y.; Christian, H.; Faust, A.; Kornberger, P.; Kohring, G.W.; Giffhorn, F.; Scheidig, A.J.
Deposited on	:	2009-09-04
Resolution	:	1.25 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:

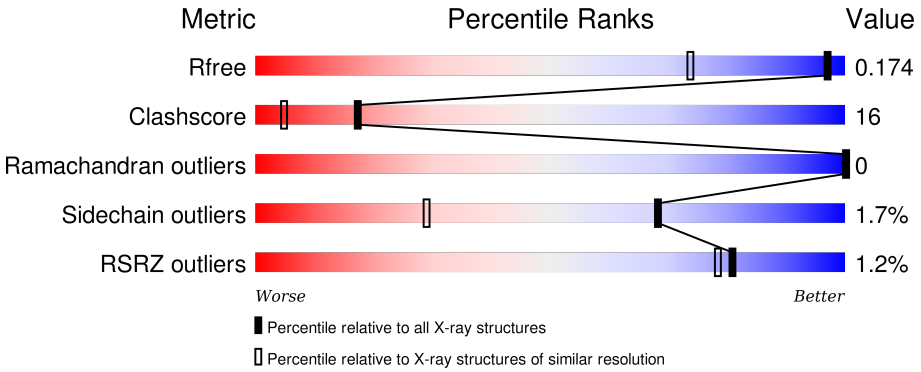
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.25 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	1442 (1.30-1.22)
Clashscore	102246	1530 (1.30-1.22)
Ramachandran outliers	100387	1467 (1.30-1.22)
Sidechain outliers	100360	1465 (1.30-1.22)
RSRZ outliers	91569	1442 (1.30-1.22)

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	254	81% 17% •
1	B	254	4% 79% 15% 5% •
1	C	254	80% 17% •
1	D	254	% 83% 13% •

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	POL	A	1255	-	-	-	X
4	POL	A	1256	-	-	-	X
4	POL	B	1255[A]	-	-	X	X
4	POL	B	1255[B]	-	-	X	X
4	POL	C	1255	-	-	-	X
4	POL	C	1256	-	-	-	X
4	POL	D	1256	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9942 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.

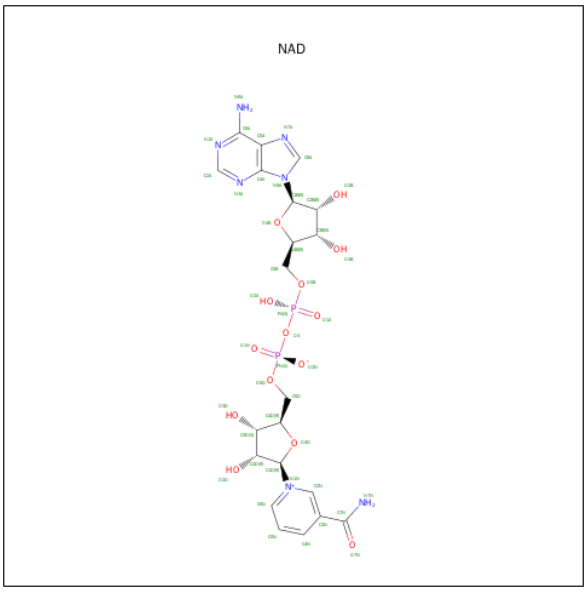
- Molecule 1 is a protein called GALACTITOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	14	0
			1968	1227	354	371	16			
1	B	254	Total	C	N	O	S	0	19	0
			2010	1249	373	371	17			
1	C	254	Total	C	N	O	S	0	18	0
			2007	1249	367	372	19			
1	D	254	Total	C	N	O	S	0	14	0
			1978	1228	366	368	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

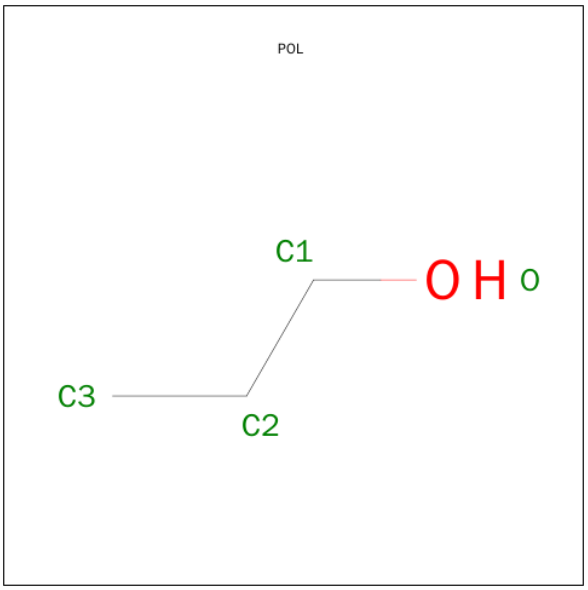
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	B	1	Total C O 8 6 2	0	1
4	B	1	Total C O 4 3 1	0	0
4	C	1	Total C O 4 3 1	0	0
4	C	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0

- Molecule 5 is water.

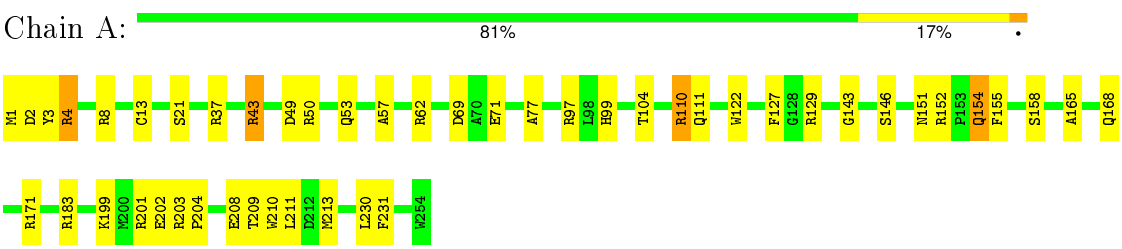
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	469	Total O 469 469	0	0
5	B	417	Total O 417 417	0	0
5	C	456	Total O 456 456	0	0
5	D	423	Total O 423 423	0	0

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.

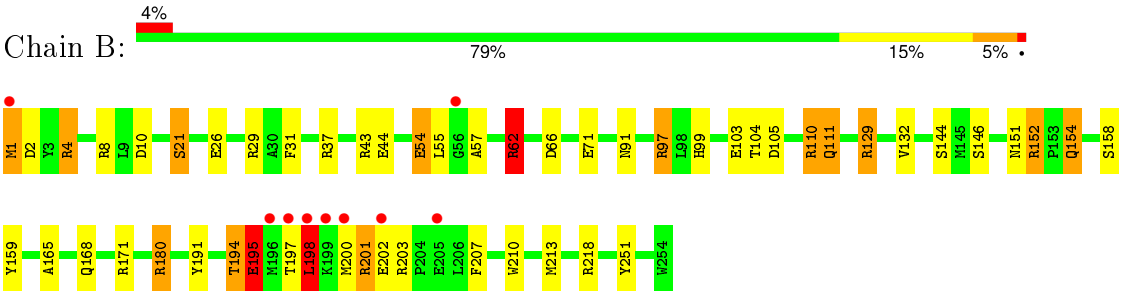
- Molecule 1: GALACTITOL DEHYDROGENASE

Chain A:



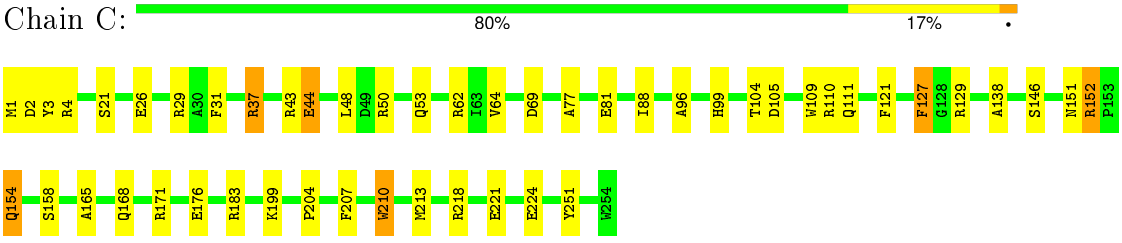
- Molecule 1: GALACTITOL DEHYDROGENASE

Chain B:



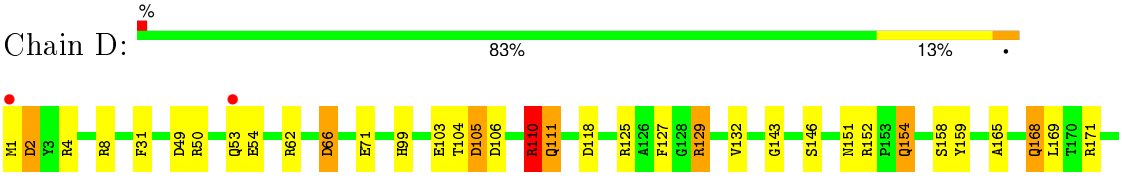
- Molecule 1: GALACTITOL DEHYDROGENASE

Chain C:



- Molecule 1: GALACTITOL DEHYDROGENASE

Chain D:




G179
R180
L198
E205
W210
M213
R218
C219
Y251
W254

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.79Å 106.62Å 109.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.25 19.94 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.94-1.25) 99.9 (19.94-1.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.134 , 0.177 0.131 , 0.174	Depositor DCC
R_{free} test set	15688 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 313320 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	9942	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, POL, NAD

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	1.45	16/2004 (0.8%)	1.33	19/2716 (0.7%)
1	B	1.55	20/2052 (1.0%)	1.57	36/2777 (1.3%)
1	C	1.47	13/2043 (0.6%)	1.53	31/2766 (1.1%)
1	D	1.42	13/2011 (0.6%)	1.45	26/2725 (1.0%)
All	All	1.47	62/8110 (0.8%)	1.47	112/10984 (1.0%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ARG	CG-CD	9.38	1.75	1.51
1	B	21	SER	CA-CB	8.84	1.66	1.52
1	B	111	GLN	CG-CD	8.40	1.70	1.51
1	C	176	GLU	CD-OE2	7.45	1.33	1.25
1	D	205	GLU	CD-OE1	7.43	1.33	1.25
1	B	54	GLU	C-O	7.42	1.37	1.23
1	C	62	ARG	CZ-NH1	7.38	1.42	1.33
1	A	110	ARG	CZ-NH2	-7.04	1.23	1.33
1	A	1	MET	CB-CG	6.92	1.73	1.51
1	B	8	ARG	CG-CD	-6.65	1.35	1.51
1	B	31	PHE	CE1-CZ	6.61	1.50	1.37
1	C	21	SER	CB-OG	6.50	1.50	1.42
1	D	50	ARG	CB-CG	-6.46	1.35	1.52
1	A	50	ARG	CG-CD	6.26	1.67	1.51
1	B	201[A]	ARG	CZ-NH1	6.18	1.41	1.33
1	B	201[B]	ARG	CZ-NH1	6.18	1.41	1.33
1	C	44[A]	GLU	CD-OE2	-6.18	1.18	1.25
1	C	44[B]	GLU	CD-OE2	-6.18	1.18	1.25
1	A	155	PHE	CD1-CE1	6.14	1.51	1.39
1	B	21	SER	CB-OG	6.13	1.50	1.42
1	C	221	GLU	CG-CD	6.03	1.60	1.51
1	A	3	TYR	CE1-CZ	6.02	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	ARG	CZ-NH1	5.89	1.40	1.33
1	A	13	CYS	CB-SG	-5.88	1.72	1.81
1	A	202	GLU	CB-CG	5.86	1.63	1.52
1	B	198	LEU	N-CA	5.77	1.57	1.46
1	C	26	GLU	CD-OE1	-5.71	1.19	1.25
1	A	49	ASP	CB-CG	5.63	1.63	1.51
1	D	127	PHE	CE2-CZ	5.58	1.48	1.37
1	C	110[A]	ARG	CZ-NH2	-5.56	1.25	1.33
1	C	110[B]	ARG	CZ-NH2	-5.56	1.25	1.33
1	C	210	TRP	CE3-CZ3	5.53	1.47	1.38
1	B	26	GLU	CG-CD	5.50	1.60	1.51
1	D	1	MET	CG-SD	5.50	1.95	1.81
1	A	231	PHE	CE2-CZ	5.46	1.47	1.37
1	A	71[A]	GLU	CD-OE2	5.45	1.31	1.25
1	A	71[B]	GLU	CD-OE2	5.45	1.31	1.25
1	A	21	SER	CA-CB	5.40	1.61	1.52
1	B	103	GLU	CD-OE2	5.34	1.31	1.25
1	D	251	TYR	CD2-CE2	5.32	1.47	1.39
1	D	50	ARG	CZ-NH2	5.30	1.40	1.33
1	D	103	GLU	CG-CD	5.28	1.59	1.51
1	B	180[A]	ARG	CB-CG	5.27	1.66	1.52
1	B	180[B]	ARG	CB-CG	5.27	1.66	1.52
1	C	50	ARG	CG-CD	5.26	1.65	1.51
1	D	219[A]	CYS	CB-SG	-5.22	1.73	1.81
1	D	219[B]	CYS	CB-SG	-5.22	1.73	1.81
1	B	91	ASN	CG-OD1	5.19	1.35	1.24
1	A	62	ARG	CG-CD	5.15	1.64	1.51
1	A	155	PHE	CE1-CZ	5.14	1.47	1.37
1	B	54	GLU	CD-OE2	-5.13	1.20	1.25
1	D	168	GLN	CD-OE1	5.12	1.35	1.24
1	C	224	GLU	CB-CG	5.12	1.61	1.52
1	B	26	GLU	CD-OE1	-5.10	1.20	1.25
1	B	8	ARG	CB-CG	5.10	1.66	1.52
1	A	203	ARG	CZ-NH1	5.09	1.39	1.33
1	B	195[A]	GLU	CD-OE2	5.09	1.31	1.25
1	B	195[B]	GLU	CD-OE2	5.09	1.31	1.25
1	D	54	GLU	CD-OE1	5.07	1.31	1.25
1	D	125	ARG	CZ-NH2	5.05	1.39	1.33
1	B	54	GLU	CD-OE1	5.05	1.31	1.25
1	C	26	GLU	CB-CG	5.04	1.61	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4[A]	ARG	NE-CZ-NH2	-19.49	110.56	120.30
1	C	4[B]	ARG	NE-CZ-NH2	-19.49	110.56	120.30
1	D	129[A]	ARG	NE-CZ-NH1	18.21	129.41	120.30
1	D	129[B]	ARG	NE-CZ-NH1	18.21	129.41	120.30
1	C	4[A]	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	C	4[B]	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	D	129[A]	ARG	NE-CZ-NH2	-15.66	112.47	120.30
1	D	129[B]	ARG	NE-CZ-NH2	-15.66	112.47	120.30
1	B	129[A]	ARG	NE-CZ-NH2	-15.43	112.59	120.30
1	B	129[B]	ARG	NE-CZ-NH2	-15.43	112.59	120.30
1	B	29[A]	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	29[B]	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	A	110	ARG	NE-CZ-NH1	-11.00	114.80	120.30
1	B	180[A]	ARG	NE-CZ-NH1	-10.45	115.07	120.30
1	B	180[B]	ARG	NE-CZ-NH1	-10.45	115.07	120.30
1	B	201[A]	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	B	201[B]	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	C	183	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	C	152[A]	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	C	152[B]	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	C	62	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	B	198	LEU	CB-CG-CD1	8.80	125.96	111.00
1	C	183	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	C	29	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	C	31	PHE	CB-CG-CD2	-8.62	114.77	120.80
1	A	8	ARG	NE-CZ-NH1	-8.55	116.02	120.30
1	B	10	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	A	2	ASP	CB-CG-OD1	8.43	125.88	118.30
1	B	97[A]	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	97[B]	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	54	GLU	O-C-N	7.71	135.03	122.70
1	B	201[A]	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	B	201[B]	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	D	66[A]	ASP	CB-CG-OD1	7.32	124.88	118.30
1	D	66[B]	ASP	CB-CG-OD1	7.32	124.88	118.30
1	D	50	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	D	8	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	129[A]	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	B	129[B]	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	183	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	31	PHE	CB-CG-CD2	-6.66	116.14	120.80
1	D	31	PHE	CB-CG-CD1	6.64	125.45	120.80
1	A	155	PHE	CD1-CE1-CZ	-6.64	112.13	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	54	GLU	CA-C-N	-6.58	102.72	117.20
1	C	4[A]	ARG	CD-NE-CZ	6.39	132.54	123.60
1	C	4[B]	ARG	CD-NE-CZ	6.39	132.54	123.60
1	C	81	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	D	66[A]	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	D	66[B]	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	B	203	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	218	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	97[A]	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	97[B]	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	97	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	37	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	B	4[A]	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	4[B]	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	152[A]	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	152[B]	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	43[A]	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	43[B]	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	66[A]	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	66[B]	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	208	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	C	2	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	43[A]	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	C	43[B]	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	C	37[A]	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	37[B]	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	211	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	D	118	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	251	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	A	122	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	C	4[A]	ARG	CG-CD-NE	-5.53	100.18	111.80
1	C	4[B]	ARG	CG-CD-NE	-5.53	100.18	111.80
1	A	69	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	4[A]	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	A	4[B]	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	C	207	PHE	CB-CG-CD2	5.45	124.61	120.80
1	B	218	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	218	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	8	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	C	109	TRP	CZ3-CH2-CZ2	5.42	128.11	121.60
1	D	105[A]	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	D	105[B]	ASP	CB-CG-OD2	-5.37	113.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	D	180[A]	ARG	CG-CD-NE	-5.30	100.67	111.80
1	D	180[B]	ARG	CG-CD-NE	-5.30	100.67	111.80
1	B	8	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	191	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	C	69	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	221	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	D	169	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	194	THR	CB-CA-C	-5.25	97.43	111.60
1	C	121	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	A	203	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	122	TRP	CB-CG-CD2	5.23	133.40	126.60
1	A	201	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	129[A]	ARG	CD-NE-CZ	5.23	130.92	123.60
1	D	129[B]	ARG	CD-NE-CZ	5.23	130.92	123.60
1	D	2	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	199	LYS	CD-CE-NZ	5.20	123.66	111.70
1	B	62[A]	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	62[B]	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	C	127	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	C	43[A]	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	C	43[B]	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	D	218	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	B	55[A]	LEU	C-N-CA	-5.04	111.72	122.30
1	B	55[B]	LEU	C-N-CA	-5.04	111.72	122.30
1	D	110[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	110[B]	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1968	0	1954	42	0
1	B	2010	0	2013	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2007	0	2004	52	0
1	D	1978	0	1967	56	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	7	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
4	A	8	0	16	1	0
4	B	12	0	23	20	0
4	C	8	0	16	2	0
4	D	8	0	16	8	0
5	A	469	0	0	13	2
5	B	417	0	0	22	1
5	C	456	0	0	17	2
5	D	423	0	0	14	1
All	All	9942	0	8113	263	3

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 16.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:CG	1:A:110:ARG:CD	1.75	1.55
1:B:198:LEU:H	1:B:198:LEU:CD2	1.29	1.38
1:B:195[B]:GLU:C	1:B:198:LEU:HD21	1.49	1.33
1:C:213[A]:MET:CE	5:D:2419:HOH:O	1.64	1.33
1:B:198:LEU:N	1:B:198:LEU:HD22	1.36	1.28
1:B:197:THR:O	1:B:201[B]:ARG:HG3	1.17	1.26
1:A:4[A]:ARG:NH1	5:A:2015:HOH:O	1.69	1.26
3:B:500:NAD:C5N	4:B:1255[B]:POL:O	1.90	1.18
1:B:198:LEU:CA	1:B:201[B]:ARG:HD3	1.76	1.15
1:C:213[A]:MET:HE2	5:D:2419:HOH:O	1.26	1.13
1:C:213[B]:MET:HE1	1:D:213[B]:MET:CE	1.78	1.11
1:A:110:ARG:NH1	5:A:2326:HOH:O	1.60	1.11
1:B:43:ARG:NH1	1:B:44[B]:GLU:OE2	1.84	1.10
1:C:152[A]:ARG:HD3	1:C:213[A]:MET:SD	1.94	1.08
1:B:110[A]:ARG:NH1	5:B:2276:HOH:O	1.71	1.07
1:B:21:SER:OG	1:B:195[A]:GLU:HG3	1.55	1.06
1:B:198:LEU:HA	1:B:201[B]:ARG:CD	1.85	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195[B]:GLU:CA	1:B:198:LEU:HD21	1.87	1.04
1:B:198:LEU:HA	1:B:201[B]:ARG:HD3	1.04	1.04
5:B:2395:HOH:O	1:C:1[B]:MET:HE3	1.57	1.04
1:B:197:THR:O	1:B:201[B]:ARG:CG	2.08	1.01
1:C:213[B]:MET:CE	1:D:213[B]:MET:HE3	1.90	1.01
1:D:111[B]:GLN:OE1	5:D:2291:HOH:O	1.76	1.00
1:B:198:LEU:H	1:B:198:LEU:HD23	1.25	1.00
1:C:213[B]:MET:HE1	1:D:213[B]:MET:HE3	1.00	1.00
1:D:71[A]:GLU:HG2	5:D:2201:HOH:O	1.59	0.99
1:B:195[B]:GLU:O	1:B:198:LEU:HD21	1.61	0.99
5:B:2395:HOH:O	1:C:1[B]:MET:CE	2.11	0.98
1:B:195[B]:GLU:O	1:B:198:LEU:CD2	2.12	0.97
1:B:195[B]:GLU:N	1:B:198:LEU:HD11	1.81	0.95
1:B:198:LEU:H	1:B:198:LEU:HD22	0.91	0.94
1:B:195[B]:GLU:CA	1:B:198:LEU:HD11	1.97	0.94
1:D:49:ASP:OD1	1:D:62[A]:ARG:NE	2.01	0.94
1:A:152:ARG:HD3	1:A:213[B]:MET:SD	2.08	0.93
1:B:195[B]:GLU:HA	1:B:198:LEU:HD21	1.47	0.93
1:B:159:TYR:OH	4:B:1255[B]:POL:H12	1.70	0.92
1:D:152[A]:ARG:HH11	1:D:213[A]:MET:CE	1.82	0.91
1:B:195[B]:GLU:HA	1:B:198:LEU:HD11	1.52	0.91
1:B:110[A]:ARG:NH1	5:B:2280:HOH:O	2.02	0.90
1:B:21:SER:HG	1:B:195[A]:GLU:HG3	1.34	0.90
1:B:1[B]:MET:CE	5:C:2432:HOH:O	2.19	0.89
1:C:204:PRO:HG3	5:C:2072:HOH:O	1.72	0.89
1:B:195[B]:GLU:HA	1:B:198:LEU:CD2	2.03	0.89
1:B:195[A]:GLU:OE2	5:B:2353:HOH:O	1.90	0.88
1:B:195[A]:GLU:C	1:B:198:LEU:HD21	1.92	0.88
1:B:201[B]:ARG:HB2	5:B:2358:HOH:O	1.74	0.88
1:B:198:LEU:N	1:B:198:LEU:CD2	2.00	0.87
1:B:110[A]:ARG:NE	5:B:2276:HOH:O	2.04	0.87
1:B:195[B]:GLU:C	1:B:198:LEU:CD2	2.41	0.86
1:B:54:GLU:HG2	5:B:2166:HOH:O	1.76	0.86
1:C:213[B]:MET:CE	1:D:213[B]:MET:CE	2.50	0.86
1:B:195[B]:GLU:HA	1:B:198:LEU:CG	2.08	0.83
1:B:195[B]:GLU:HA	1:B:198:LEU:CD1	2.08	0.83
1:B:1[B]:MET:HE2	5:C:2432:HOH:O	1.76	0.82
1:B:154:GLN:HE21	1:B:154:GLN:H	1.28	0.81
1:C:152[A]:ARG:HD3	1:C:213[A]:MET:CE	2.10	0.80
1:C:105[B]:ASP:OD1	5:C:2293:HOH:O	1.99	0.79
1:A:37[A]:ARG:NH1	1:A:57:ALA:O	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:NH1	1:B:213[B]:MET:HE2	1.99	0.78
1:B:159:TYR:CZ	4:B:1255[B]:POL:H12	2.21	0.76
1:D:105[A]:ASP:OD1	5:D:2273:HOH:O	2.04	0.76
1:C:152[B]:ARG:NH2	5:C:2346:HOH:O	2.18	0.76
1:C:111[B]:GLN:NE2	5:C:2312:HOH:O	2.18	0.76
1:D:154:GLN:H	1:D:154:GLN:HE21	1.33	0.75
3:B:500:NAD:C6N	4:B:1255[B]:POL:O	2.35	0.75
1:D:152[A]:ARG:HH11	1:D:213[A]:MET:HE1	1.51	0.74
1:B:1[A]:MET:HE1	5:B:2112:HOH:O	1.87	0.74
1:A:37[B]:ARG:HD3	5:A:2135:HOH:O	1.87	0.74
1:C:154:GLN:HE22	1:C:210:TRP:HE1	1.35	0.74
1:B:144:SER:OG	4:B:1255[B]:POL:H11	1.88	0.74
1:B:194:THR:O	1:B:198:LEU:CD1	2.36	0.74
1:A:199[B]:LYS:NZ	5:A:2401:HOH:O	2.22	0.73
1:C:213[A]:MET:HE1	5:D:2419:HOH:O	1.54	0.72
3:B:500:NAD:C4N	4:B:1255[B]:POL:O	2.37	0.72
1:B:152[A]:ARG:NH2	5:B:2308:HOH:O	2.22	0.72
1:B:146:SER:OG	4:B:1255[B]:POL:H33	1.89	0.72
1:B:195[A]:GLU:HA	1:B:198:LEU:HD11	1.71	0.72
1:C:154:GLN:H	1:C:154:GLN:HE21	1.38	0.71
1:B:195[B]:GLU:O	1:B:198:LEU:HD23	1.90	0.71
1:C:152[A]:ARG:CD	1:C:213[A]:MET:SD	2.78	0.70
1:B:159:TYR:CE2	4:B:1255[B]:POL:H12	2.25	0.70
1:A:154:GLN:HE21	1:A:154:GLN:H	1.38	0.70
4:B:1255[A]:POL:H22	4:B:1256:POL:H12	1.73	0.70
1:B:154:GLN:HE22	1:B:210:TRP:HE1	1.39	0.70
1:B:194:THR:C	1:B:198:LEU:HD11	2.12	0.70
1:D:105[B]:ASP:OD1	5:D:2269:HOH:O	2.09	0.70
1:B:197:THR:HG22	4:B:1255[A]:POL:H32	1.75	0.69
1:C:213[B]:MET:CE	1:D:152[B]:ARG:NH1	2.55	0.69
1:D:152[A]:ARG:HD3	1:D:213[A]:MET:CE	2.23	0.68
1:C:152[A]:ARG:HD3	1:C:213[A]:MET:HE3	1.75	0.68
1:A:43[A]:ARG:NH1	5:A:2146:HOH:O	2.27	0.68
1:B:146:SER:HG	4:B:1255[B]:POL:H33	1.59	0.68
1:B:194:THR:C	1:B:198:LEU:CD1	2.63	0.67
1:C:99:HIS:HD2	1:C:104:THR:OG1	1.77	0.67
1:B:154:GLN:NE2	1:B:154:GLN:H	1.92	0.67
1:D:152[A]:ARG:NE	5:D:2317:HOH:O	2.27	0.67
1:A:37[A]:ARG:CZ	1:A:57:ALA:O	2.43	0.66
1:D:154:GLN:HE22	1:D:210:TRP:HE1	1.42	0.66
1:C:53[B]:GLN:NE2	5:C:2158:HOH:O	2.17	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:NE2	5:A:2194:HOH:O	2.29	0.66
1:A:110:ARG:NE	1:A:110:ARG:CG	2.57	0.65
1:D:99:HIS:HD2	1:D:104:THR:OG1	1.78	0.65
1:D:152[A]:ARG:NH2	5:D:2316:HOH:O	2.28	0.64
1:C:213[B]:MET:HE3	1:D:152[B]:ARG:NH1	2.12	0.64
1:D:62[A]:ARG:NH1	5:D:2170:HOH:O	2.28	0.64
1:B:159:TYR:OH	4:B:1255[B]:POL:C1	2.46	0.64
1:B:180[B]:ARG:HD2	5:B:2330:HOH:O	1.96	0.64
1:C:44[B]:GLU:OE2	5:C:2137:HOH:O	2.15	0.63
1:C:146:SER:HG	4:C:1255:POL:H21	1.64	0.63
1:A:154:GLN:NE2	1:A:154:GLN:H	1.97	0.63
1:B:97[B]:ARG:NH2	1:B:111:GLN:HG2	2.13	0.63
1:B:197:THR:HG22	4:B:1255[A]:POL:C3	2.29	0.63
1:D:154:GLN:H	1:D:154:GLN:NE2	1.97	0.62
1:B:201[A]:ARG:HG2	1:B:207:PHE:CE1	2.33	0.62
1:C:213[B]:MET:HA	1:C:213[B]:MET:HE3	1.81	0.62
1:D:159:TYR:OH	4:D:1256:POL:C1	2.47	0.62
1:B:194:THR:O	1:B:198:LEU:CD2	2.48	0.61
1:B:105[B]:ASP:OD1	5:B:2269:HOH:O	2.16	0.61
1:D:152[A]:ARG:HD3	1:D:213[A]:MET:HE3	1.82	0.61
1:C:154:GLN:H	1:C:154:GLN:NE2	1.98	0.61
1:B:1[A]:MET:CG	5:C:2432:HOH:O	2.48	0.60
1:D:159:TYR:CZ	4:D:1256:POL:H11	2.36	0.60
1:B:195[A]:GLU:N	1:B:198:LEU:HD11	2.17	0.60
1:A:213[B]:MET:HE1	5:A:2356:HOH:O	2.01	0.60
1:A:152:ARG:NH1	1:B:213[B]:MET:CE	2.64	0.60
1:B:194:THR:O	1:B:198:LEU:HD13	2.02	0.59
1:D:49:ASP:OD1	1:D:62[A]:ARG:CZ	2.50	0.59
1:B:110[A]:ARG:CZ	5:B:2276:HOH:O	2.13	0.59
1:C:129[B]:ARG:NH1	5:C:2327:HOH:O	2.35	0.59
1:A:152:ARG:HH12	1:B:213[B]:MET:HE2	1.68	0.58
1:B:1[A]:MET:HG3	5:C:2432:HOH:O	2.02	0.58
1:D:152[A]:ARG:HH11	1:D:213[A]:MET:HE3	1.64	0.58
1:B:197:THR:C	1:B:201[B]:ARG:HG3	2.15	0.58
1:D:152[A]:ARG:NH1	1:D:213[A]:MET:CE	2.61	0.58
1:B:4[A]:ARG:NH2	5:B:2022:HOH:O	2.35	0.58
1:C:213[B]:MET:HE1	1:D:152[B]:ARG:NH1	2.17	0.58
1:B:99:HIS:HD2	1:B:104:THR:OG1	1.87	0.57
1:A:152:ARG:HH12	1:B:213[B]:MET:CE	2.17	0.57
1:B:57[A]:ALA:HB1	5:B:2168:HOH:O	2.04	0.57
1:A:99:HIS:HD2	1:A:104:THR:OG1	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152[A]:ARG:HG2	5:D:2317:HOH:O	2.04	0.57
1:D:129[B]:ARG:NH1	5:D:2299:HOH:O	2.30	0.57
1:A:110:ARG:CB	1:A:110:ARG:CD	2.76	0.56
1:A:37[A]:ARG:NH2	1:A:57:ALA:O	2.38	0.56
1:B:159:TYR:CE2	4:B:1255[B]:POL:C1	2.88	0.56
1:B:201[B]:ARG:HA	1:B:207:PHE:CD1	2.41	0.56
1:B:198:LEU:HD13	1:B:201[A]:ARG:NH2	2.21	0.56
1:B:195[A]:GLU:CA	1:B:198:LEU:HD11	2.33	0.55
5:B:2395:HOH:O	1:C:1[B]:MET:HE2	1.91	0.55
1:B:195[A]:GLU:CG	3:B:500:NAD:O2A	2.55	0.55
1:B:195[A]:GLU:HG3	3:B:500:NAD:O2A	2.07	0.55
1:B:151:ASN:HD22	1:B:151:ASN:H	1.55	0.55
1:A:154:GLN:HE22	1:A:210:TRP:HE1	1.54	0.54
1:D:159:TYR:CE2	4:D:1256:POL:H11	2.42	0.54
1:A:129:ARG:NH1	5:A:2339:HOH:O	2.06	0.54
1:C:1[B]:MET:SD	1:C:3:TYR:CE1	3.00	0.54
1:A:151:ASN:HD22	1:A:151:ASN:H	1.54	0.53
1:D:151:ASN:H	1:D:151:ASN:HD22	1.56	0.53
3:B:500:NAD:O7N	4:B:1255[A]:POL:H33	2.08	0.53
1:A:152:ARG:CD	1:A:213[B]:MET:SD	2.90	0.53
1:D:2:ASP:OD1	1:D:4[A]:ARG:HB2	2.09	0.53
1:D:146:SER:OG	4:D:1256:POL:H33	2.08	0.53
1:B:159:TYR:HE2	4:B:1255[B]:POL:C1	2.22	0.52
1:B:198:LEU:N	1:B:201[B]:ARG:HD3	2.24	0.52
1:C:213[B]:MET:CE	1:D:213[B]:MET:SD	2.98	0.52
1:B:110[A]:ARG:CZ	1:B:110[A]:ARG:HA	2.40	0.51
1:B:195[A]:GLU:CA	1:B:198:LEU:HD21	2.34	0.51
1:C:37[A]:ARG:HH21	1:C:37[A]:ARG:HG2	1.75	0.51
1:C:213[B]:MET:CE	1:D:152[B]:ARG:HH12	2.24	0.51
1:A:110:ARG:HD3	5:A:2143:HOH:O	2.10	0.51
1:B:1[B]:MET:HE1	5:C:2432:HOH:O	1.99	0.50
1:C:154:GLN:NE2	1:C:210:TRP:HE1	2.04	0.50
1:B:201[A]:ARG:HA	1:B:207:PHE:CD1	2.46	0.50
1:C:1[B]:MET:HE1	5:C:2439:HOH:O	2.11	0.50
1:C:99:HIS:HE1	1:C:158:SER:OG	1.95	0.50
1:B:54:GLU:CG	5:B:2166:HOH:O	2.45	0.49
5:A:2356:HOH:O	1:B:213[B]:MET:HE2	2.12	0.49
1:C:48[A]:LEU:HD12	1:C:64:VAL:HG22	1.94	0.49
1:D:132:VAL:HG13	1:D:180[B]:ARG:HD2	1.94	0.49
1:B:197:THR:C	1:B:198:LEU:HD22	2.21	0.49
1:D:159:TYR:HH	4:D:1256:POL:C1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLN:HE22	1:C:171:ARG:HE	1.60	0.49
1:D:179:GLY:C	1:D:180[A]:ARG:HG3	2.32	0.49
1:C:151:ASN:HD22	1:C:151:ASN:H	1.60	0.49
1:C:204:PRO:CG	5:C:2072:HOH:O	2.45	0.49
1:D:154:GLN:NE2	1:D:210:TRP:HE1	2.10	0.49
1:B:154:GLN:NE2	1:B:210:TRP:HE1	2.06	0.49
1:D:105[B]:ASP:O	1:D:106:ASP:C	2.51	0.49
1:A:209:THR:O	1:A:213[B]:MET:HG3	2.12	0.48
1:C:111[A]:GLN:OE1	5:C:2311:HOH:O	2.20	0.48
1:A:37[B]:ARG:CD	5:A:2135:HOH:O	2.54	0.48
1:B:99:HIS:HE1	1:B:158:SER:OG	1.97	0.48
1:C:213[B]:MET:HE2	1:D:213[B]:MET:SD	2.53	0.48
5:B:2280:HOH:O	1:D:110[A]:ARG:NH2	2.46	0.48
1:B:99:HIS:CE1	1:B:158:SER:H	2.32	0.48
1:B:1[A]:MET:HG2	5:C:2432:HOH:O	2.12	0.48
1:A:152:ARG:HH11	1:B:213[B]:MET:HE2	1.78	0.47
1:B:144:SER:OG	4:B:1255[B]:POL:C1	2.61	0.47
1:B:201[A]:ARG:HG2	1:B:207:PHE:CD1	2.49	0.47
1:A:154:GLN:NE2	1:A:210:TRP:HE1	2.11	0.47
1:B:198:LEU:HD13	1:B:201[B]:ARG:NH1	2.29	0.47
1:A:204:PRO:HG2	5:A:2093:HOH:O	2.13	0.47
1:D:168:GLN:HE22	1:D:171:ARG:HE	1.63	0.47
1:B:198:LEU:HD13	1:B:201[A]:ARG:HH22	1.79	0.47
1:C:99:HIS:CD2	1:C:104:THR:OG1	2.65	0.47
1:A:168:GLN:HE22	1:A:171:ARG:HE	1.62	0.47
1:B:62[B]:ARG:O	1:B:62[B]:ARG:HG3	2.14	0.47
1:B:201[A]:ARG:CG	1:B:207:PHE:CE1	2.98	0.47
1:D:152[A]:ARG:NH1	1:D:213[A]:MET:HE3	2.27	0.47
1:B:213[B]:MET:HA	1:B:213[B]:MET:CE	2.45	0.46
1:B:57[A]:ALA:CB	5:B:2168:HOH:O	2.60	0.46
1:D:110[A]:ARG:NH2	5:D:2285:HOH:O	2.45	0.46
1:D:159:TYR:OH	4:D:1256:POL:H11	2.16	0.46
1:B:129[B]:ARG:NH1	5:B:2293:HOH:O	2.48	0.46
1:C:96:ALA:HB1	4:C:1256:POL:H31	1.98	0.46
1:C:1[B]:MET:CE	5:C:2439:HOH:O	2.64	0.46
1:B:197:THR:CG2	4:B:1255[A]:POL:C3	2.93	0.45
1:B:201[A]:ARG:HG2	1:B:207:PHE:HE1	1.77	0.45
1:B:71:GLU:HG3	5:B:2204:HOH:O	2.15	0.45
1:B:97[B]:ARG:HH22	1:B:111:GLN:HG2	1.80	0.45
1:B:159:TYR:HE2	4:B:1255[B]:POL:H11	1.80	0.45
1:B:202:GLU:HG3	5:B:2358:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:HIS:HE1	1:A:158:SER:OG	2.00	0.45
1:A:4[A]:ARG:NH2	5:A:2021:HOH:O	2.49	0.45
1:C:99:HIS:CE1	1:C:158:SER:H	2.34	0.45
1:B:165:ALA:HB2	1:D:165:ALA:HB2	1.99	0.45
1:D:146:SER:OG	4:D:1256:POL:C3	2.65	0.45
1:D:4[B]:ARG:NE	5:D:2028:HOH:O	2.48	0.44
1:D:99:HIS:CE1	1:D:158:SER:H	2.35	0.44
1:A:99:HIS:CE1	1:A:158:SER:H	2.36	0.44
1:B:197:THR:OG1	1:B:201[B]:ARG:HD2	2.16	0.44
1:A:146:SER:OG	4:A:1256:POL:C3	2.66	0.44
1:B:168:GLN:HE22	1:B:171:ARG:HE	1.65	0.43
1:C:99:HIS:CE1	1:C:158:SER:OG	2.71	0.43
1:B:99:HIS:HE1	1:B:158:SER:H	1.67	0.43
1:A:99:HIS:HE1	1:A:158:SER:H	1.65	0.43
1:C:77:ALA:HA	1:C:127:PHE:CE1	2.54	0.43
1:B:198:LEU:HD13	1:B:201[B]:ARG:HH11	1.83	0.43
1:A:77:ALA:HA	1:A:127:PHE:CE1	2.54	0.43
1:D:99:HIS:HE1	1:D:158:SER:OG	2.02	0.42
1:B:2:ASP:OD1	1:B:4[B]:ARG:HB2	2.20	0.42
1:D:143:GLY:O	3:D:500:NAD:H6N	2.20	0.42
1:D:146:SER:HG	4:D:1256:POL:H33	1.83	0.42
1:A:165:ALA:HB2	1:C:165:ALA:HB2	2.01	0.42
1:B:21:SER:OG	1:B:195[A]:GLU:CG	2.46	0.42
1:D:99:HIS:CD2	1:D:104:THR:OG1	2.66	0.42
1:A:111[B]:GLN:HE21	1:A:111[B]:GLN:HA	1.85	0.42
1:B:213[B]:MET:HA	1:B:213[B]:MET:HE2	2.01	0.42
1:B:99:HIS:CE1	1:B:158:SER:OG	2.72	0.41
1:A:99:HIS:CE1	1:A:158:SER:OG	2.73	0.41
1:C:213[B]:MET:HB2	1:C:251:TYR:CE1	2.56	0.41
3:B:500:NAD:C4N	4:B:1255[A]:POL:H11	2.50	0.41
1:D:66[B]:ASP:OD2	3:D:500:NAD:N6A	2.53	0.41
1:B:110[A]:ARG:HH21	1:B:110[A]:ARG:HB2	1.85	0.41
1:B:200:MET:HB3	1:B:210:TRP:CH2	2.55	0.41
1:B:213[B]:MET:HB3	1:B:251:TYR:CE1	2.55	0.41
1:B:197:THR:C	1:B:201[B]:ARG:CG	2.83	0.40
1:B:132:VAL:HG13	1:B:180[A]:ARG:HD2	2.03	0.40
1:B:194:THR:C	1:B:198:LEU:HD13	2.38	0.40
1:A:143:GLY:O	3:A:500:NAD:H6N	2.21	0.40
1:B:197:THR:C	1:B:201[B]:ARG:CD	2.89	0.40
1:C:88:ILE:HA	1:C:138:ALA:O	2.21	0.40
1:B:194:THR:O	1:B:198:LEU:CG	2.70	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2208:HOH:O	5:C:2144:HOH:O[3_655]	1.99	0.21
5:A:2089:HOH:O	5:B:2362:HOH:O[3_655]	2.04	0.16
5:C:2068:HOH:O	5:D:2215:HOH:O[2_674]	2.12	0.08

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	266/254 (105%)	262 (98%)	4 (2%)	0	100	100
1	B	270/254 (106%)	266 (98%)	4 (2%)	0	100	100
1	C	269/254 (106%)	264 (98%)	5 (2%)	0	100	100
1	D	266/254 (105%)	264 (99%)	2 (1%)	0	100	100
All	All	1071/1016 (105%)	1056 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	188/174 (108%)	187 (100%)	1 (0%)	92	72
1	B	191/174 (110%)	181 (95%)	10 (5%)	29	2
1	C	192/174 (110%)	191 (100%)	1 (0%)	92	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	188/174 (108%)	182 (97%)	6 (3%)	46 8
All	All	759/696 (109%)	741 (98%)	18 (2%)	68 15

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	B	1[A]	MET
1	B	1[B]	MET
1	B	62[A]	ARG
1	B	62[B]	ARG
1	B	110[A]	ARG
1	B	110[B]	ARG
1	B	154	GLN
1	B	195[A]	GLU
1	B	195[B]	GLU
1	B	198	LEU
1	C	154	GLN
1	D	53	GLN
1	D	110[A]	ARG
1	D	110[B]	ARG
1	D	111[A]	GLN
1	D	111[B]	GLN
1	D	154	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	99	HIS
1	A	154	GLN
1	A	168	GLN
1	B	53	GLN
1	B	91	ASN
1	B	99	HIS
1	B	151	ASN
1	B	154	GLN
1	B	168	GLN
1	C	91	ASN
1	C	99	HIS
1	C	154	GLN

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Mol	Chain	Res	Type
1	C	168	GLN
1	D	53	GLN
1	D	91	ASN
1	D	99	HIS
1	D	154	GLN
1	D	168	GLN

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

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	POL	A	1255	-	3,3,3	0.66	0	2,2,2	0.86	0
4	POL	A	1256	-	3,3,3	1.42	1 (33%)	2,2,2	2.40	1 (50%)
3	NAD	A	500	-	38,48,48	1.81	7 (18%)	47,73,73	2.24	8 (17%)
4	POL	B	1255[A]	-	3,3,3	0.58	0	2,2,2	1.15	0
4	POL	B	1255[B]	-	3,3,3	1.53	1 (33%)	2,2,2	0.55	0
4	POL	B	1256	-	3,3,3	0.33	0	2,2,2	0.51	0
3	NAD	B	500	-	38,48,48	1.20	4 (10%)	47,73,73	2.53	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	POL	C	1255	-	3,3,3	1.55	1 (33%)	2,2,2	2.14	1 (50%)
4	POL	C	1256	-	3,3,3	0.46	0	2,2,2	1.09	0
3	NAD	C	500	-	38,48,48	1.74	5 (13%)	47,73,73	2.17	8 (17%)
4	POL	D	1255	-	3,3,3	0.19	0	2,2,2	0.98	0
4	POL	D	1256	-	3,3,3	1.12	0	2,2,2	2.64	1 (50%)
3	NAD	D	500	-	38,48,48	1.28	4 (10%)	47,73,73	1.33	7 (14%)

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	POL	A	1255	-	-	0/1/1/1	0/0/0/0
4	POL	A	1256	-	-	0/1/1/1	0/0/0/0
3	NAD	A	500	-	-	0/22/62/62	0/5/5/5
4	POL	B	1255[A]	-	-	0/1/1/1	0/0/0/0
4	POL	B	1255[B]	-	-	0/1/1/1	0/0/0/0
4	POL	B	1256	-	-	0/1/1/1	0/0/0/0
3	NAD	B	500	-	-	0/22/62/62	0/5/5/5
4	POL	C	1255	-	-	0/1/1/1	0/0/0/0
4	POL	C	1256	-	-	0/1/1/1	0/0/0/0
3	NAD	C	500	-	-	0/22/62/62	0/5/5/5
4	POL	D	1255	-	-	0/1/1/1	0/0/0/0
4	POL	D	1256	-	-	0/1/1/1	0/0/0/0
3	NAD	D	500	-	-	0/22/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	NAD	C3N-C7N	-4.05	1.44	1.50
3	A	500	NAD	C2N-C3N	-2.58	1.35	1.39
4	B	1255[B]	POL	O-C1	-2.51	1.28	1.42
3	A	500	NAD	C3N-C7N	-2.18	1.47	1.50
3	B	500	NAD	C2N-C3N	2.04	1.42	1.39
3	D	500	NAD	C2A-N1A	2.04	1.37	1.33
3	A	500	NAD	C4A-N3A	2.11	1.38	1.35
3	B	500	NAD	C5N-C4N	2.17	1.43	1.38
4	A	1256	POL	O-C1	2.25	1.54	1.42
4	C	1255	POL	O-C1	2.57	1.55	1.42
3	D	500	NAD	C2A-N3A	2.64	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	O4B-C4B	2.79	1.51	1.45
3	B	500	NAD	O7N-C7N	2.91	1.30	1.24
3	B	500	NAD	C2A-N3A	3.17	1.37	1.32
3	C	500	NAD	C6N-N1N	3.19	1.44	1.35
3	D	500	NAD	C4N-C3N	3.33	1.45	1.39
3	C	500	NAD	C4N-C3N	3.34	1.45	1.39
3	A	500	NAD	C6N-N1N	3.38	1.44	1.35
3	C	500	NAD	C2A-N3A	3.86	1.39	1.32
3	D	500	NAD	O7N-C7N	3.95	1.32	1.24
3	A	500	NAD	O4B-C1B	4.81	1.47	1.41
3	C	500	NAD	O7N-C7N	5.85	1.36	1.24
3	A	500	NAD	O7N-C7N	5.94	1.36	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	500	NAD	N3A-C2A-N1A	-10.85	120.58	128.89
3	B	500	NAD	N3A-C2A-N1A	-10.44	120.90	128.89
3	A	500	NAD	O7N-C7N-C3N	-6.55	112.43	119.59
3	B	500	NAD	O7N-C7N-C3N	-4.87	114.27	119.59
3	B	500	NAD	C3N-C2N-N1N	-4.65	115.00	120.36
3	D	500	NAD	C1B-N9A-C4A	-3.54	121.60	126.94
4	A	1256	POL	C3-C2-C1	-3.36	73.26	114.24
3	A	500	NAD	N3A-C2A-N1A	-3.33	126.34	128.89
4	D	1256	POL	O-C1-C2	-3.16	77.77	112.77
3	A	500	NAD	O7N-C7N-N7N	-3.15	118.16	122.59
3	D	500	NAD	N3A-C2A-N1A	-3.14	126.49	128.89
4	C	1255	POL	C3-C2-C1	-3.01	77.47	114.24
3	C	500	NAD	C5N-C4N-C3N	-2.90	116.69	120.33
3	B	500	NAD	C1B-N9A-C4A	-2.89	122.58	126.94
3	A	500	NAD	C4B-O4B-C1B	-2.77	106.68	109.72
3	C	500	NAD	O7N-C7N-N7N	-2.68	118.83	122.59
3	A	500	NAD	C1B-N9A-C4A	-2.66	122.93	126.94
3	D	500	NAD	O3D-C3D-C2D	-2.41	103.98	111.83
3	C	500	NAD	C4N-C3N-C7N	-2.27	115.08	121.09
3	D	500	NAD	C2B-C1B-N9A	-2.27	110.82	114.29
3	D	500	NAD	C3N-C2N-N1N	-2.13	117.91	120.36
3	A	500	NAD	O4B-C4B-C5B	-2.05	101.98	109.32
3	C	500	NAD	O4D-C1D-N1N	2.41	110.78	108.13
3	C	500	NAD	C2A-N1A-C6A	2.42	123.08	118.77
3	D	500	NAD	O4D-C1D-N1N	2.64	111.03	108.13
3	C	500	NAD	C3N-C2N-N1N	2.92	123.73	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	500	NAD	C3N-C7N-N7N	2.99	121.09	117.82
3	A	500	NAD	C2N-C3N-C4N	3.82	122.54	118.29
3	B	500	NAD	C2A-N1A-C6A	4.43	126.69	118.77
3	C	500	NAD	C3N-C7N-N7N	5.06	123.36	117.82
3	B	500	NAD	C2N-C3N-C4N	5.37	124.27	118.29
3	B	500	NAD	C3N-C7N-N7N	7.01	125.49	117.82
3	A	500	NAD	C3N-C7N-N7N	10.50	129.31	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1256	POL	1	0
3	A	500	NAD	1	0
4	B	1255[A]	POL	6	0
4	B	1255[B]	POL	14	0
4	B	1256	POL	1	0
3	B	500	NAD	7	0
4	C	1255	POL	1	0
4	C	1256	POL	1	0
4	D	1256	POL	8	0
3	D	500	NAD	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	254/254 (100%)	-0.49	0 100 100	10, 16, 25, 30	0
1	B	254/254 (100%)	-0.37	9 (3%) 48 40	10, 15, 32, 51	0
1	C	254/254 (100%)	-0.53	0 100 100	10, 16, 27, 36	0
1	D	254/254 (100%)	-0.43	3 (1%) 81 78	11, 17, 30, 48	1 (0%)
All	All	1016/1016 (100%)	-0.45	12 (1%) 81 78	10, 16, 28, 51	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	LYS	5.4
1	B	1[A]	MET	4.0
1	B	198	LEU	3.3
1	D	1	MET	3.2
1	B	200	MET	3.2
1	B	196	MET	2.8
1	B	202	GLU	2.7
1	B	56[A]	GLY	2.5
1	D	53	GLN	2.4
1	B	205	GLU	2.2
1	B	197	THR	2.1
1	D	198	LEU	2.1

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

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

6.3 Carbohydrates

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	POL	B	1255[B]	4/4	0.64	0.42	32.63	11,11,16,22	4
4	POL	A	1256	4/4	0.81	0.16	14.21	15,20,23,29	0
4	POL	C	1255	4/4	0.88	0.14	11.78	15,20,24,27	0
4	POL	D	1256	4/4	0.86	0.14	11.61	15,21,25,31	0
4	POL	A	1255	4/4	0.81	0.16	5.68	40,41,42,48	0
4	POL	B	1255[A]	4/4	0.64	0.42	4.72	26,26,26,28	4
4	POL	C	1256	4/4	0.93	0.09	2.38	30,33,36,38	0
4	POL	B	1256	4/4	0.80	0.14	1.70	34,37,39,39	0
4	POL	D	1255	4/4	0.93	0.10	1.55	36,38,38,40	0
3	NAD	B	500	44/44	0.97	0.05	-0.50	12,16,18,20	0
3	NAD	A	500	44/44	0.98	0.04	-0.54	11,14,16,17	0
3	NAD	D	500	44/44	0.98	0.04	-0.78	13,18,20,22	0
3	NAD	C	500	44/44	0.98	0.04	-0.79	12,15,18,20	0
2	MG	C	256	1/1	1.00	0.04	-1.62	12,12,12,12	0
2	MG	A	256	1/1	1.00	0.03	-3.11	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.