



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:13 PM GMT

PDB ID : 1GD1  
Title : STRUCTURE OF HOLO-GLYCERALDEHYDE-3-PHOSPHATE-DEHYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS AT 1.8 ANGSTROMS RESOLUTION  
Authors : Skarzynski, T.; Moody, P.C.E.; Wonacott, A.J.  
Deposited on : 1987-06-22  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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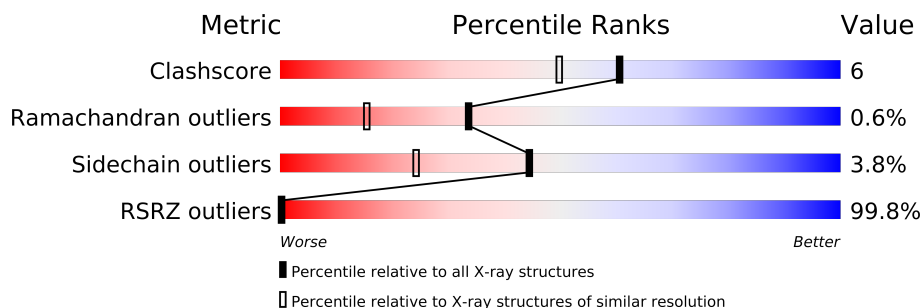
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	O	334	
1	P	334	
1	Q	334	
1	R	334	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10984 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HOLO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			
1	P	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			
1	Q	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			
1	R	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



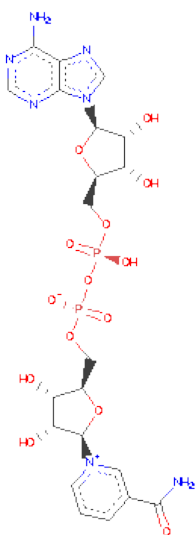
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	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	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

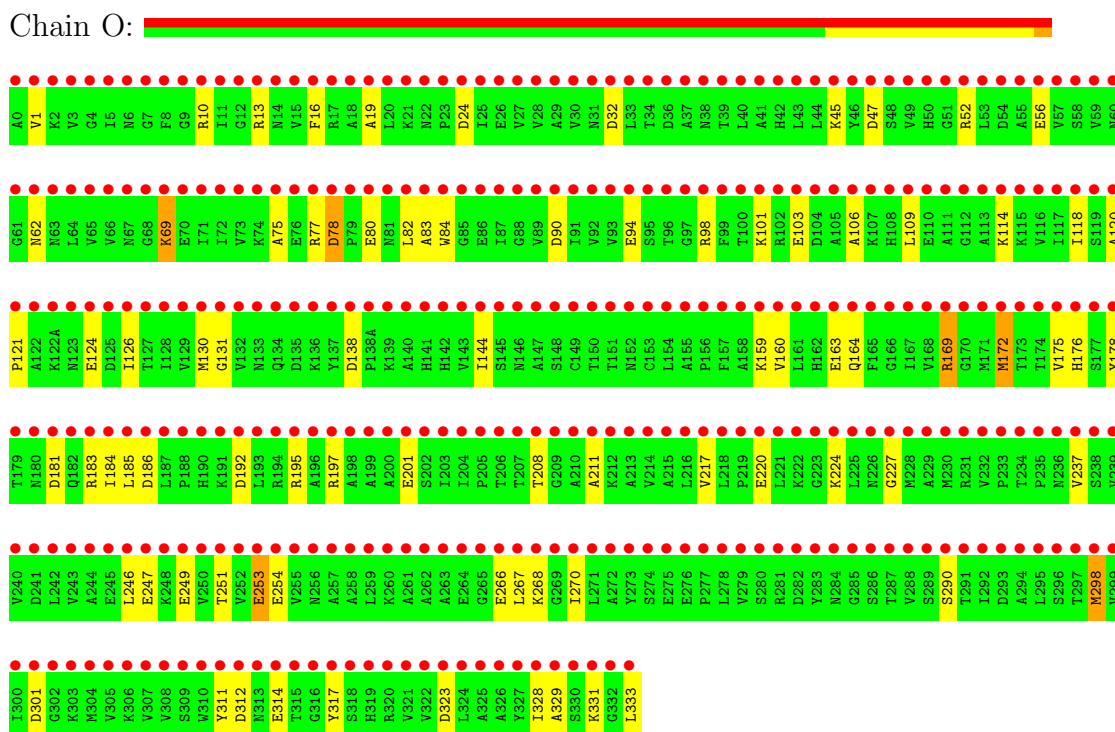
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	176	Total 176	O 176	0	0
4	P	162	Total 162	O 162	0	0
4	Q	166	Total 166	O 166	0	0
4	R	164	Total 164	O 164	0	0

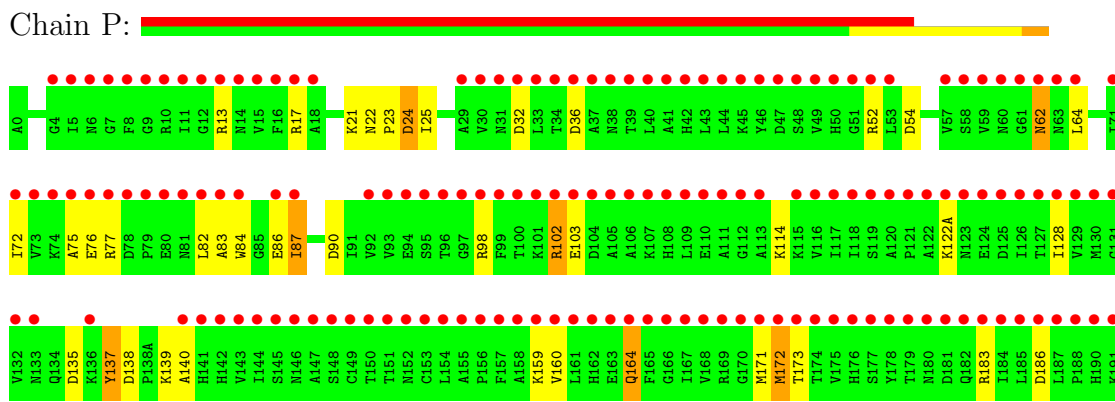
### 3 Residue-property plots

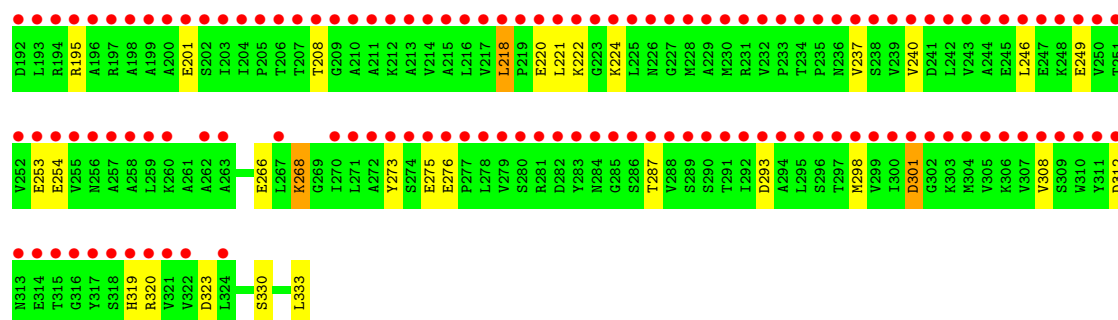
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE



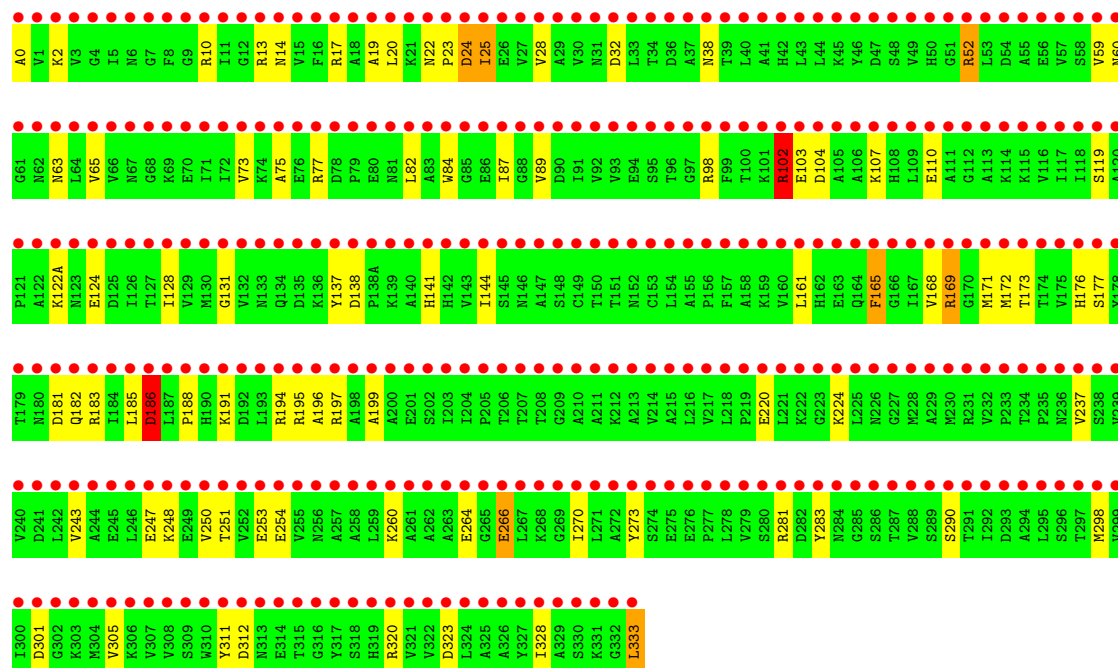
#### • Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE





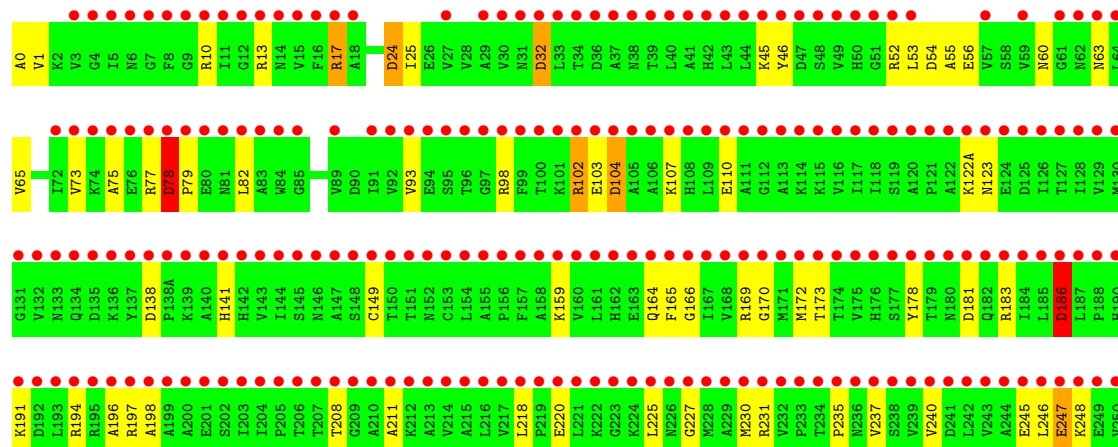
● Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

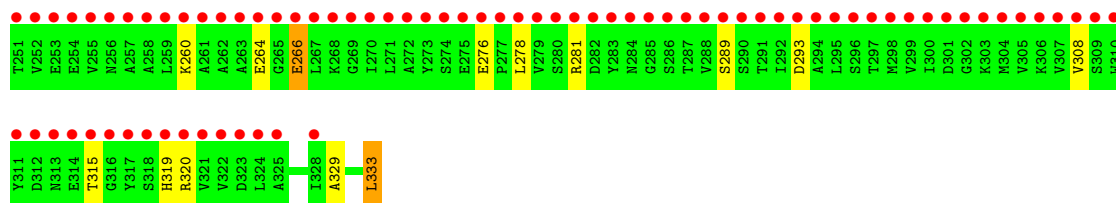
Chain Q:



● Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

Chain R:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.44Å 124.10Å 82.54Å 90.00° 108.98° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80 18.81 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 79.8 (18.81-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.177 , (Not available) 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.81 , 451.4	EDS
Estimated twinning fraction	0.137 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 116031 reflections	Xtriage
$F_o, F_c$ correlation	0.28	EDS
Total number of atoms	10984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	O	1.06	1/2561 (0.0%)	1.83	55/3474 (1.6%)
1	P	1.09	0/2561	1.76	42/3474 (1.2%)
1	Q	1.07	0/2561	1.85	59/3474 (1.7%)
1	R	1.07	2/2561 (0.1%)	1.81	43/3474 (1.2%)
All	All	1.07	3/10244 (0.0%)	1.81	199/13896 (1.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	178	TYR	CE1-CZ	5.21	1.45	1.38
1	R	78	ASP	CG-OD2	5.18	1.37	1.25
1	R	289	SER	CA-CB	5.05	1.60	1.52

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	266	GLU	CA-CB-CG	18.23	153.49	113.40
1	O	98	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	P	98	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	Q	98	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	R	98	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	O	10	ARG	NE-CZ-NH1	17.14	128.87	120.30
1	O	98	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	P	98	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	Q	98	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	R	98	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	R	10	ARG	NE-CZ-NH1	15.35	127.97	120.30
1	R	183	ARG	NE-CZ-NH1	14.41	127.51	120.30
1	Q	13	ARG	NE-CZ-NH2	12.45	126.52	120.30
1	Q	10	ARG	NE-CZ-NH1	11.87	126.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	320	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	O	197	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	R	17	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	O	197	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	P	102	ARG	NE-CZ-NH1	-10.70	114.95	120.30
1	Q	161	LEU	CB-CG-CD2	10.69	129.17	111.00
1	Q	312	ASP	CB-CG-OD1	10.59	127.83	118.30
1	P	135	ASP	CB-CG-OD1	10.54	127.79	118.30
1	O	10	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	P	312	ASP	CB-CG-OD1	10.36	127.62	118.30
1	O	195	ARG	NE-CZ-NH2	10.18	125.39	120.30
1	R	266	GLU	CA-CB-CG	9.96	135.31	113.40
1	P	301	ASP	CB-CG-OD1	9.82	127.14	118.30
1	Q	323	ASP	CB-CG-OD1	9.75	127.08	118.30
1	Q	183	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	R	231	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	R	231	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	O	183	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	Q	197	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	P	301	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	Q	13	ARG	CD-NE-CZ	9.17	136.44	123.60
1	P	13	ARG	CD-NE-CZ	8.98	136.18	123.60
1	R	264	GLU	OE1-CD-OE2	8.98	134.08	123.30
1	Q	194	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	P	13	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	Q	52	ARG	NE-CZ-NH2	8.61	124.60	120.30
1	Q	281	ARG	NE-CZ-NH1	-8.53	116.03	120.30
1	R	10	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	P	36	ASP	CB-CG-OD1	8.51	125.96	118.30
1	O	169	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	P	201	GLU	OE1-CD-OE2	8.42	133.40	123.30
1	Q	104	ASP	CB-CG-OD1	8.41	125.87	118.30
1	P	266	GLU	CB-CG-CD	8.25	136.47	114.20
1	P	17	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	Q	17	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	O	201	GLU	OE1-CD-OE2	8.08	133.00	123.30
1	Q	183	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	O	47	ASP	O-C-N	8.01	135.52	122.70
1	R	32	ASP	CB-CG-OD1	7.99	125.49	118.30
1	R	104	ASP	CB-CG-OD1	7.98	125.48	118.30
1	O	312	ASP	CB-CG-OD1	7.92	125.43	118.30
1	R	13	ARG	CD-NE-CZ	7.70	134.38	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	138	ASP	CB-CG-OD1	7.52	125.07	118.30
1	P	17	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	Q	301	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	P	266	GLU	OE1-CD-OE2	-7.49	114.31	123.30
1	O	323	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	O	77	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	Q	102	ARG	CB-CA-C	7.41	125.23	110.40
1	Q	323	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	Q	311	TYR	CB-CG-CD2	7.40	125.44	121.00
1	R	102	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	Q	169	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	R	78	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	Q	281	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	O	301	ASP	CB-CG-OD1	7.15	124.73	118.30
1	R	194	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	O	195	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	R	181	ASP	CB-CG-OD1	7.06	124.65	118.30
1	R	52	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	Q	283	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	P	173	THR	N-CA-CB	6.91	123.44	110.30
1	Q	77	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	P	17	ARG	CD-NE-CZ	6.87	133.21	123.60
1	O	311	TYR	CB-CG-CD2	6.83	125.10	121.00
1	Q	181	ASP	CB-CG-OD1	6.79	124.42	118.30
1	R	186	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	P	64	LEU	CA-CB-CG	6.73	130.78	115.30
1	O	24	ASP	CB-CG-OD1	6.72	124.34	118.30
1	O	253	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	Q	124	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	R	54	ASP	CB-CG-OD1	6.64	124.28	118.30
1	Q	197	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	O	169	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	P	140	ALA	N-CA-CB	-6.52	100.97	110.10
1	O	78	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	P	54	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	O	323	ASP	CB-CG-OD1	6.40	124.06	118.30
1	O	77	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	R	173	THR	N-CA-CB	6.31	122.28	110.30
1	R	198	ALA	CB-CA-C	6.30	119.55	110.10
1	P	137	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	R	293	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	P	13	ARG	NH1-CZ-NH2	-6.23	112.54	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	290	SER	N-CA-CB	-6.23	101.15	110.50
1	P	320	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	Q	77	ARG	CA-CB-CG	6.22	127.08	113.40
1	O	176	HIS	N-CA-CB	-6.21	99.41	110.60
1	P	24	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	Q	161	LEU	CA-CB-CG	6.18	129.50	115.30
1	R	24	ASP	CB-CG-OD1	6.18	123.86	118.30
1	Q	290	SER	N-CA-CB	-6.14	101.29	110.50
1	Q	173	THR	N-CA-CB	6.11	121.90	110.30
1	Q	195	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	R	93	VAL	O-C-N	6.10	132.45	122.70
1	Q	266	GLU	CG-CD-OE1	6.09	130.47	118.30
1	R	169	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	O	80	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	P	195	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	Q	312	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	Q	52	ARG	CD-NE-CZ	6.00	132.00	123.60
1	O	47	ASP	CA-C-N	-6.00	104.00	117.20
1	O	124	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	R	46	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	P	276	GLU	OE1-CD-OE2	5.98	130.47	123.30
1	O	298	MET	CA-CB-CG	5.97	123.45	113.30
1	R	230	MET	CA-CB-CG	-5.96	103.17	113.30
1	O	314	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	R	149	CYS	CB-CA-C	5.93	122.25	110.40
1	P	273	TYR	CB-CG-CD2	-5.92	117.44	121.00
1	R	264	GLU	CG-CD-OE2	-5.91	106.47	118.30
1	Q	102	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	Q	102	ARG	N-CA-CB	-5.90	99.97	110.60
1	O	314	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	Q	281	ARG	N-CA-CB	5.87	121.16	110.60
1	P	102	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	Q	298	MET	N-CA-CB	-5.81	100.14	110.60
1	Q	24	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	P	138	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	Q	186	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	R	56	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	O	130	MET	CG-SD-CE	-5.65	91.16	100.20
1	R	178	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	P	293	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	O	13	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	R	245	GLU	OE1-CD-OE2	5.61	130.03	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	183	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	O	80	GLU	CG-CD-OE2	-5.59	107.11	118.30
1	O	90	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	O	317	TYR	CG-CD2-CE2	-5.59	116.83	121.30
1	Q	176	HIS	N-CA-CB	-5.58	100.55	110.60
1	Q	52	ARG	CG-CD-NE	5.57	123.50	111.80
1	O	52	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	P	298	MET	N-CA-CB	-5.52	100.67	110.60
1	Q	17	ARG	CD-NE-CZ	5.51	131.32	123.60
1	O	333	LEU	CA-CB-CG	5.51	127.98	115.30
1	R	32	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	R	247	GLU	CB-CG-CD	5.49	129.03	114.20
1	Q	171	MET	N-CA-CB	5.48	120.47	110.60
1	Q	250	VAL	O-C-N	5.48	131.47	122.70
1	P	195	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	O	178	TYR	CD1-CE1-CZ	-5.46	114.88	119.80
1	Q	110	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	R	56	GLU	CG-CD-OE2	-5.43	107.44	118.30
1	P	218	LEU	CA-C-O	5.42	131.49	120.10
1	P	275	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	R	104	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	R	13	ARG	O-C-N	5.32	131.21	122.70
1	P	266	GLU	CG-CD-OE1	5.30	128.90	118.30
1	Q	253	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	Q	77	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	Q	199	ALA	CB-CA-C	-5.27	102.20	110.10
1	P	52	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	P	253	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	P	323	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	O	13	ARG	CD-NE-CZ	5.23	130.93	123.60
1	O	178	TYR	CG-CD1-CE1	5.23	125.48	121.30
1	R	55	ALA	O-C-N	5.21	131.03	122.70
1	Q	194	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	Q	110	GLU	CB-CG-CD	5.19	128.22	114.20
1	R	77	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	O	138	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	O	78	ASP	OD1-CG-OD2	5.18	133.13	123.30
1	Q	266	GLU	CB-CG-CD	5.17	128.17	114.20
1	R	183	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	R	197	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	O	192	ASP	CB-CG-OD1	5.17	122.95	118.30
1	Q	14	ASN	CB-CA-C	5.15	120.70	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	195	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	P	102	ARG	CG-CD-NE	-5.12	101.04	111.80
1	O	130	MET	N-CA-CB	-5.11	101.41	110.60
1	O	181	ASP	CB-CG-OD1	5.10	122.89	118.30
1	Q	320	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	O	175	VAL	N-CA-C	-5.09	97.26	111.00
1	O	298	MET	CB-CA-C	5.08	120.56	110.40
1	Q	273	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	P	254	GLU	OE1-CD-OE2	5.07	129.39	123.30
1	O	249	GLU	CA-CB-CG	5.07	124.56	113.40
1	O	217	VAL	C-N-CA	5.06	134.35	121.70
1	O	253	GLU	CG-CD-OE1	5.05	128.41	118.30
1	Q	177	SER	O-C-N	5.05	130.79	122.70
1	O	101	LYS	CA-CB-CG	5.04	124.50	113.40
1	O	181	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	O	126	ILE	O-C-N	5.03	130.75	122.70
1	P	287	THR	CA-CB-CG2	5.01	119.41	112.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2525	0	2572	26	0
1	P	2525	0	2572	24	0
1	Q	2525	0	2572	38	0
1	R	2525	0	2572	36	0
2	O	10	0	0	0	0
2	P	10	0	0	1	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	O	44	0	26	0	0
3	P	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	44	0	26	1	0
3	R	44	0	26	0	0
4	O	176	0	0	5	0
4	P	162	0	0	3	0
4	Q	166	0	0	2	0
4	R	164	0	0	4	0
All	All	10984	0	10392	122	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:102:ARG:HH11	1:Q:102:ARG:HG3	1.38	0.89
1:Q:220:GLU:CD	1:Q:220:GLU:H	1.89	0.76
1:Q:102:ARG:HG3	1:Q:102:ARG:NH1	2.07	0.69
1:O:16:PHE:HA	4:O:434:HOH:O	1.91	0.69
1:R:172:MET:CE	1:R:208:THR:HG21	2.24	0.68
1:P:76:GLU:OE2	4:P:425:HOH:O	2.14	0.66
1:Q:102:ARG:CG	1:Q:102:ARG:NH1	2.58	0.64
1:Q:60:ASN:HB2	1:Q:65:VAL:CG2	2.28	0.63
1:P:172:MET:CE	1:P:208:THR:HG21	2.29	0.63
1:O:144:ILE:HD13	1:O:328:ILE:HD11	1.82	0.62
1:R:329:ALA:HA	1:R:333:LEU:HD22	1.82	0.62
1:R:165:PHE:HA	1:R:248:LYS:HD2	1.84	0.60
1:R:122(A):LYS:O	1:R:123:ASN:HB2	2.01	0.60
1:Q:168:VAL:CG2	1:Q:247:GLU:HG3	2.32	0.60
1:R:0:ALA:HB3	1:R:24:ASP:O	2.02	0.59
1:Q:144:ILE:HD13	1:Q:328:ILE:HD11	1.84	0.59
1:O:266:GLU:HG3	1:O:267:LEU:HG	1.85	0.58
1:Q:22:ASN:OD1	1:Q:24:ASP:HB2	2.04	0.58
1:P:83:ALA:HB1	1:P:86:GLU:OE2	2.03	0.57
1:Q:128:ILE:HD11	1:Q:137:TYR:HB2	1.85	0.57
1:Q:0:ALA:HB3	1:Q:24:ASP:O	2.05	0.57
1:Q:191:LYS:HG2	4:Q:432:HOH:O	2.05	0.56
1:O:19:ALA:HB3	4:O:434:HOH:O	2.07	0.55
1:P:114:LYS:HD2	1:P:333:LEU:HG	1.88	0.55
1:Q:144:ILE:HD13	1:Q:328:ILE:CD1	2.37	0.55
1:O:251:THR:OG1	1:O:254:GLU:HG3	2.08	0.54
1:Q:19:ALA:CB	1:Q:25:ILE:HD11	2.38	0.54
1:Q:19:ALA:HB1	1:Q:25:ILE:HD11	1.90	0.54
1:R:107:LYS:HA	1:R:110:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:224:LYS:NZ	4:P:464:HOH:O	2.28	0.53
1:R:220:GLU:CD	1:R:220:GLU:H	2.11	0.53
1:Q:60:ASN:HB2	1:Q:65:VAL:HG23	1.89	0.53
1:O:172:MET:CE	1:O:208:THR:HG21	2.38	0.53
1:O:172:MET:HG3	1:O:227:GLY:HA3	1.91	0.53
1:R:191:LYS:HG2	4:R:429:HOH:O	2.08	0.53
1:R:172:MET:HE1	1:R:208:THR:HG21	1.90	0.51
1:P:159:LYS:HB2	1:P:218:LEU:HD11	1.91	0.51
1:Q:165:PHE:O	1:Q:248:LYS:HG3	2.11	0.51
1:O:224:LYS:NZ	4:O:471:HOH:O	2.41	0.50
1:P:240:VAL:O	1:P:308:VAL:HA	2.12	0.50
1:O:45:LYS:HG2	4:O:401:HOH:O	2.11	0.50
1:P:128:ILE:HD11	1:P:137:TYR:HB2	1.93	0.49
1:O:131:GLY:HA3	1:O:270:ILE:HD13	1.93	0.49
1:O:144:ILE:HD13	1:O:328:ILE:CD1	2.42	0.49
1:O:298:MET:HG2	1:P:171:MET:CE	2.43	0.49
1:P:160:VAL:O	1:P:164:GLN:HB2	2.13	0.49
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.48	0.48
1:R:164:GLN:NE2	4:R:444:HOH:O	2.47	0.48
1:R:1:VAL:CG1	1:R:25:ILE:HG22	2.44	0.47
1:O:169:ARG:HD3	1:P:301:ASP:HB2	1.96	0.47
1:P:90:ASP:OD1	1:P:114:LYS:HE3	2.14	0.47
1:R:78:ASP:HB2	4:R:433:HOH:O	2.13	0.47
1:Q:182:GLN:HB3	4:Q:374:HOH:O	2.14	0.47
1:R:60:ASN:HB2	1:R:65:VAL:CG2	2.44	0.47
1:R:186:ASP:HA	1:R:196:ALA:O	2.14	0.47
1:R:172:MET:HG2	1:R:211:ALA:HB2	1.95	0.47
1:R:45:LYS:HE3	1:R:45:LYS:HB2	1.69	0.47
1:R:172:MET:HE2	1:R:208:THR:HG21	1.96	0.46
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.50	0.46
1:Q:60:ASN:HB2	1:Q:65:VAL:HG21	1.98	0.46
1:O:106:ALA:O	1:O:109:LEU:HB2	2.16	0.46
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.51	0.46
1:O:69:LYS:H	1:O:69:LYS:HG2	1.60	0.45
1:P:102:ARG:HG3	1:P:102:ARG:NH1	2.31	0.45
1:P:32:ASP:O	1:P:75:ALA:HA	2.17	0.45
1:O:1:VAL:HG21	1:O:329:ALA:HB1	1.98	0.45
1:R:138:ASP:N	1:R:141:HIS:ND1	2.61	0.45
1:R:103:GLU:HG3	1:R:104:ASP:N	2.32	0.45
1:P:72:ILE:HD13	1:P:87:ILE:HG21	1.99	0.44
1:P:21:LYS:HE2	1:P:319:HIS:HE1	1.81	0.44
1:R:79:PRO:HA	1:R:82:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:333:LEU:HD12	1:Q:333:LEU:HA	1.84	0.44
1:R:276:GLU:HB2	1:R:278:LEU:HG	2.00	0.44
1:Q:38:ASN:HD21	1:Q:59:VAL:HG11	1.83	0.43
1:R:172:MET:HG3	1:R:227:GLY:HA3	2.00	0.43
1:Q:22:ASN:OD1	1:Q:23:PRO:HD2	2.19	0.43
1:O:82:LEU:O	1:O:83:ALA:HB3	2.19	0.43
4:P:368:HOH:O	1:Q:188:PRO:HD3	2.19	0.43
1:Q:38:ASN:ND2	1:Q:59:VAL:HG11	2.33	0.43
1:O:32:ASP:O	1:O:75:ALA:HA	2.19	0.43
1:R:17:ARG:HG2	1:R:53:LEU:CD1	2.48	0.43
1:R:159:LYS:HB2	1:R:218:LEU:HD11	2.01	0.43
1:R:315:THR:O	1:R:319:HIS:HD2	2.02	0.43
1:Q:32:ASP:O	1:Q:75:ALA:HA	2.19	0.42
1:P:77:ARG:HD2	1:P:77:ARG:HH11	1.69	0.42
1:Q:131:GLY:HA3	1:Q:270:ILE:HD13	2.02	0.42
1:P:221:LEU:O	1:P:222:LYS:C	2.58	0.42
1:O:172:MET:HG2	1:O:211:ALA:HB2	2.01	0.42
1:O:120:ALA:HB1	1:O:121:PRO:CD	2.50	0.42
1:O:159:LYS:O	1:O:163:GLU:HG3	2.19	0.42
1:R:281:ARG:HB3	1:R:281:ARG:HE	1.67	0.42
1:R:17:ARG:HG2	1:R:53:LEU:HD13	2.01	0.42
1:R:166:GLY:HA3	1:R:247:GLU:HG3	2.01	0.42
1:Q:63:ASN:ND2	1:Q:73:VAL:H	2.17	0.42
1:Q:138:ASP:N	1:Q:141:HIS:ND1	2.50	0.42
1:R:60:ASN:HB2	1:R:65:VAL:HG21	2.01	0.42
1:Q:2:LYS:HE2	1:Q:28:VAL:HG11	2.02	0.42
1:Q:251:THR:OG1	1:Q:254:GLU:N	2.49	0.42
1:R:102:ARG:HD3	1:R:102:ARG:HH11	1.59	0.42
1:O:184:ILE:HG22	1:O:185:LEU:HG	2.01	0.41
1:R:63:ASN:ND2	1:R:73:VAL:H	2.18	0.41
1:P:139:LYS:HA	1:P:139:LYS:HD2	1.80	0.41
1:P:268:LYS:HB2	1:P:268:LYS:HE3	1.88	0.41
1:Q:186:ASP:HA	1:Q:196:ALA:O	2.20	0.41
1:Q:169:ARG:HA	1:Q:224:LYS:O	2.20	0.41
1:P:62:ASN:HD22	1:P:62:ASN:HA	1.59	0.41
1:Q:243:VAL:HA	1:Q:305:VAL:O	2.20	0.41
1:O:160:VAL:O	1:O:164:GLN:HB2	2.21	0.41
1:Q:119:SER:O	3:Q:336:NAD:H6N	2.19	0.41
1:P:22:ASN:OD1	1:P:24:ASP:HB2	2.20	0.41
1:Q:185:LEU:O	1:Q:186:ASP:C	2.59	0.41
1:Q:20:LEU:HA	1:Q:20:LEU:HD23	1.91	0.41
1:P:208:THR:OG1	2:P:339:SO4:O3	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:79:PRO:HA	1:R:82:LEU:CD1	2.51	0.41
1:O:94:GLU:HB3	1:O:118:ILE:HA	2.03	0.41
1:R:32:ASP:O	1:R:75:ALA:HA	2.21	0.41
1:R:240:VAL:O	1:R:308:VAL:HA	2.21	0.41
1:Q:260:LYS:NZ	1:Q:264:GLU:OE2	2.51	0.41
1:Q:87:ILE:HG13	1:Q:89:VAL:HG23	2.03	0.41
1:R:170:GLY:O	1:R:225:LEU:HA	2.21	0.40
1:O:114:LYS:HD2	4:O:485:HOH:O	2.20	0.40
1:R:17:ARG:NE	4:R:421:HOH:O	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	332/334 (99%)	314 (95%)	16 (5%)	2 (1%)	33	15
1	P	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	33	15
1	Q	332/334 (99%)	316 (95%)	14 (4%)	2 (1%)	33	15
1	R	332/334 (99%)	318 (96%)	12 (4%)	2 (1%)	33	15
All	All	1328/1336 (99%)	1263 (95%)	57 (4%)	8 (1%)	33	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	186	ASP
1	O	237	VAL
1	P	237	VAL
1	Q	186	ASP
1	Q	237	VAL
1	R	186	ASP
1	R	237	VAL
1	O	186	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	272/272 (100%)	260 (96%)	12 (4%)	39	18
1	P	272/272 (100%)	259 (95%)	13 (5%)	35	15
1	Q	272/272 (100%)	262 (96%)	10 (4%)	45	26
1	R	272/272 (100%)	266 (98%)	6 (2%)	64	48
All	All	1088/1088 (100%)	1047 (96%)	41 (4%)	44	24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	56	GLU
1	O	62	ASN
1	O	69	LYS
1	O	78	ASP
1	O	103	GLU
1	O	172	MET
1	O	220	GLU
1	O	246	LEU
1	O	247	GLU
1	O	253	GLU
1	O	268	LYS
1	O	331	LYS
1	P	23	PRO
1	P	25	ILE
1	P	62	ASN
1	P	87	ILE
1	P	103	GLU
1	P	122(A)	LYS
1	P	164	GLN
1	P	172	MET
1	P	220	GLU
1	P	246	LEU
1	P	249	GLU
1	P	268	LYS
1	P	330	SER
1	Q	25	ILE

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Mol	Chain	Res	Type
1	Q	52	ARG
1	Q	102	ARG
1	Q	103	GLU
1	Q	107	LYS
1	Q	122(A)	LYS
1	Q	165	PHE
1	Q	172	MET
1	Q	266	GLU
1	Q	333	LEU
1	R	78	ASP
1	R	235	PRO
1	R	246	LEU
1	R	260	LYS
1	R	266	GLU
1	R	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	62	ASN
1	O	81	ASN
1	O	146	ASN
1	O	152	ASN
1	O	256	ASN
1	P	62	ASN
1	P	63	ASN
1	P	146	ASN
1	P	152	ASN
1	P	256	ASN
1	Q	38	ASN
1	Q	63	ASN
1	Q	152	ASN
1	Q	256	ASN
1	Q	319	HIS
1	R	63	ASN
1	R	146	ASN
1	R	152	ASN
1	R	256	ASN
1	R	319	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAD	O	336	-	48,48,48	1.09	4 (8%)	73,73,73	1.78	12 (16%)
2	SO4	O	338	-	4,4,4	1.05	0	6,6,6	0.47	0
2	SO4	O	339	-	4,4,4	1.93	1 (25%)	6,6,6	1.16	1 (16%)
3	NAD	P	336	-	48,48,48	1.26	5 (10%)	73,73,73	1.68	15 (20%)
2	SO4	P	338	-	4,4,4	0.79	0	6,6,6	0.51	0
2	SO4	P	339	-	4,4,4	1.72	2 (50%)	6,6,6	0.40	0
3	NAD	Q	336	-	48,48,48	1.29	5 (10%)	73,73,73	1.93	14 (19%)
2	SO4	Q	338	-	4,4,4	1.31	1 (25%)	6,6,6	0.82	0
2	SO4	Q	339	-	4,4,4	1.78	1 (25%)	6,6,6	0.65	0
3	NAD	R	336	-	48,48,48	1.12	3 (6%)	73,73,73	1.99	14 (19%)
2	SO4	R	338	-	4,4,4	0.91	0	6,6,6	0.44	0
2	SO4	R	339	-	4,4,4	1.80	1 (25%)	6,6,6	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	O	336	-	-	0/30/62/62	0/3/5/5
2	SO4	O	338	-	-	0/0/0/0	0/0/0/0
2	SO4	O	339	-	-	0/0/0/0	0/0/0/0
3	NAD	P	336	-	-	0/30/62/62	0/3/5/5
2	SO4	P	338	-	-	0/0/0/0	0/0/0/0
2	SO4	P	339	-	-	0/0/0/0	0/0/0/0
3	NAD	Q	336	-	-	0/30/62/62	0/3/5/5
2	SO4	Q	338	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	339	-	-	0/0/0/0	0/0/0/0
3	NAD	R	336	-	-	0/30/62/62	0/3/5/5
2	SO4	R	338	-	-	0/0/0/0	0/0/0/0
2	SO4	R	339	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	336	NAD	C3N-C7N	4.68	1.58	1.50
3	P	336	NAD	C3N-C7N	4.13	1.57	1.50
3	R	336	NAD	C3N-C7N	4.05	1.57	1.50
3	O	336	NAD	C3N-C7N	3.56	1.56	1.50
3	P	336	NAD	PA-O3	-3.54	1.53	1.59
3	R	336	NAD	PN-O3	-3.11	1.54	1.60
3	Q	336	NAD	PN-O2N	-2.98	1.41	1.48
2	Q	339	SO4	O1-S	2.93	1.56	1.47
2	O	339	SO4	O1-S	2.73	1.56	1.47
2	R	339	SO4	O4-S	2.67	1.56	1.47
3	Q	336	NAD	O4B-C1B	2.67	1.45	1.41
3	O	336	NAD	PN-O3	-2.58	1.55	1.60
3	Q	336	NAD	O4B-C4B	2.46	1.50	1.45
3	O	336	NAD	C6N-N1N	2.35	1.42	1.35
3	P	336	NAD	O4B-C1B	2.33	1.44	1.41
3	O	336	NAD	PA-O3	-2.33	1.55	1.59
3	P	336	NAD	PN-O2N	-2.28	1.43	1.48
2	P	339	SO4	O4-S	2.27	1.55	1.47
3	R	336	NAD	C4N-C3N	2.24	1.43	1.39
2	Q	338	SO4	O2-S	2.12	1.54	1.47
2	P	339	SO4	O1-S	2.07	1.53	1.47
3	Q	336	NAD	PN-O3	-2.04	1.56	1.60
3	P	336	NAD	PA-O1A	-2.01	1.43	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	336	NAD	O4B-C1B-N9A	-8.08	100.92	108.44
3	R	336	NAD	O4B-C1B-N9A	-7.37	101.59	108.44
3	R	336	NAD	O7N-C7N-C3N	-6.13	112.67	119.58
3	O	336	NAD	O4B-C1B-N9A	-6.06	102.80	108.44
3	P	336	NAD	O4B-C1B-N9A	-5.43	103.39	108.44
3	R	336	NAD	C5N-C4N-C3N	-5.17	113.61	120.32
3	Q	336	NAD	N3A-C2A-N1A	-4.89	124.62	128.71
3	O	336	NAD	C5N-C6N-N1N	-4.80	112.34	120.43
3	Q	336	NAD	C4N-C3N-C7N	-4.73	108.52	121.10
3	Q	336	NAD	C2N-C3N-C4N	4.66	123.59	118.31
3	R	336	NAD	C4N-C3N-C7N	-4.59	108.90	121.10
3	P	336	NAD	C4B-O4B-C1B	-4.50	104.86	109.75
3	R	336	NAD	C2N-C3N-C4N	4.17	123.04	118.31
3	O	336	NAD	C4N-C3N-C7N	-4.16	110.04	121.10
3	R	336	NAD	C6N-C5N-C4N	4.06	125.88	119.44
3	O	336	NAD	C6N-C5N-C4N	4.00	125.80	119.44
3	P	336	NAD	C4N-C3N-C7N	-3.83	110.91	121.10
3	O	336	NAD	C3N-C7N-N7N	3.82	122.11	117.77
3	O	336	NAD	C6N-N1N-C2N	3.79	126.32	122.04
3	Q	336	NAD	C5N-C6N-N1N	-3.49	114.55	120.43
3	O	336	NAD	C5N-C4N-C3N	-3.36	115.95	120.32
3	P	336	NAD	C2N-C3N-C4N	3.34	122.10	118.31
3	Q	336	NAD	O7N-C7N-C3N	-3.33	115.82	119.58
3	Q	336	NAD	C4B-O4B-C1B	-3.17	106.30	109.75
3	P	336	NAD	C5N-C4N-C3N	-3.16	116.22	120.32
3	O	336	NAD	C2N-C3N-C4N	3.11	121.83	118.31
3	R	336	NAD	C4A-C5A-N7A	3.08	112.16	109.52
3	Q	336	NAD	C5N-C4N-C3N	-3.06	116.34	120.32
3	P	336	NAD	O4D-C1D-N1N	-3.06	104.82	107.95
3	R	336	NAD	C5N-C6N-N1N	-3.04	115.31	120.43
3	Q	336	NAD	C2A-N1A-C6A	2.98	124.15	118.77
3	O	336	NAD	C2N-C3N-C7N	2.95	128.13	119.35
3	P	336	NAD	C5N-C6N-N1N	-2.93	115.49	120.43
3	P	336	NAD	C4A-C5A-N7A	2.92	112.02	109.52
3	R	336	NAD	C2N-C3N-C7N	2.88	127.91	119.35
3	Q	336	NAD	C2N-C3N-C7N	2.87	127.89	119.35
3	Q	336	NAD	C6N-C5N-C4N	2.82	123.92	119.44
3	R	336	NAD	O7N-C7N-N7N	2.75	126.57	122.59
2	O	339	SO4	O2-S-O1	-2.73	100.50	109.53
3	R	336	NAD	N6A-C6A-N1A	2.72	124.70	119.36
3	P	336	NAD	C6N-C5N-C4N	2.68	123.70	119.44
3	Q	336	NAD	O7N-C7N-N7N	2.65	126.43	122.59
3	R	336	NAD	C3N-C7N-N7N	2.63	120.76	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	336	NAD	O7N-C7N-C3N	-2.62	116.62	119.58
3	O	336	NAD	O3D-C3D-C4D	-2.60	103.43	111.08
3	P	336	NAD	C2N-C3N-C7N	2.55	126.94	119.35
3	P	336	NAD	C1B-N9A-C4A	-2.50	122.31	126.64
3	Q	336	NAD	C6N-N1N-C2N	2.47	124.83	122.04
3	R	336	NAD	C4B-O4B-C1B	-2.37	107.17	109.75
3	P	336	NAD	C6N-N1N-C2N	2.36	124.70	122.04
3	P	336	NAD	O2A-PA-O5B	-2.25	97.19	108.51
3	Q	336	NAD	C3N-C2N-N1N	-2.15	116.73	120.36
3	O	336	NAD	O2D-C2D-C1D	-2.14	104.77	111.23
3	P	336	NAD	O4D-C1D-C2D	-2.09	103.57	106.77
3	P	336	NAD	C8A-N9A-C1B	2.07	130.46	126.38
3	R	336	NAD	O3-PN-O1N	2.01	113.62	108.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	334/334 (100%)	10.90	334 (100%) 0 0	4, 14, 37, 55	0
1	P	283/334 (84%)	12.46	283 (100%) 0 0	3, 14, 33, 52	0
1	Q	334/334 (100%)	12.01	334 (100%) 0 0	4, 16, 43, 59	0
1	R	301/334 (90%)	11.97	299 (99%) 0 0	4, 14, 34, 60	0
All	All	1252/1336 (93%)	11.81	1250 (99%) 0 0	3, 14, 38, 60	0

All (1250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	4	GLY	34.4
1	P	87	ILE	34.4
1	P	140	ALA	34.1
1	O	157	PHE	33.1
1	Q	11	ILE	30.2
1	Q	12	GLY	29.9
1	R	265	GLY	29.7
1	O	106	ALA	29.3
1	R	27	VAL	29.0
1	P	317	TYR	29.0
1	Q	294	ALA	28.8
1	P	161	LEU	28.7
1	P	147	ALA	28.4
1	O	215	ALA	28.0
1	P	144	ILE	27.8
1	P	223	GLY	27.4
1	Q	250	VAL	27.4
1	P	29	ALA	27.3
1	R	43	LEU	26.6
1	R	157	PHE	26.4
1	Q	308	VAL	26.2

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Mol	Chain	Res	Type	RSRZ
1	Q	75	ALA	26.1
1	P	92	VAL	26.0
1	Q	1	VAL	25.9
1	P	215	ALA	25.8
1	R	15	VAL	25.5
1	Q	300	ILE	25.4
1	P	302	GLY	25.2
1	P	72	ILE	24.9
1	R	72	ILE	24.8
1	Q	149	CYS	24.7
1	P	271	LEU	24.5
1	Q	117	ILE	24.5
1	R	118	ILE	23.9
1	Q	145	SER	23.9
1	R	75	ALA	23.8
1	O	221	LEU	23.5
1	Q	252	VAL	23.5
1	P	239	VAL	23.3
1	O	292	ILE	23.3
1	P	61	GLY	23.2
1	R	158	ALA	23.2
1	O	105	ALA	23.1
1	R	117	ILE	23.1
1	Q	88	GLY	23.0
1	Q	317	TYR	23.0
1	Q	0	ALA	22.8
1	Q	311	TYR	22.7
1	R	305	VAL	22.6
1	P	12	GLY	22.6
1	Q	30	VAL	22.5
1	R	29	ALA	22.5
1	R	11	ILE	22.5
1	Q	19	ALA	22.4
1	R	258	ALA	22.4
1	O	127	THR	22.3
1	P	49	VAL	22.2
1	O	83	ALA	22.1
1	O	160	VAL	22.1
1	R	5	ILE	22.0
1	P	115	LYS	21.9
1	P	41	ALA	21.8
1	R	127	THR	21.8

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Mol	Chain	Res	Type	RSRZ
1	O	165	PHE	21.8
1	O	185	LEU	21.8
1	Q	73	VAL	21.8
1	O	242	LEU	21.6
1	P	240	VAL	21.6
1	O	126	ILE	21.6
1	Q	148	SER	21.6
1	Q	33	LEU	21.5
1	R	299	VAL	21.5
1	R	4	GLY	21.5
1	P	59	VAL	21.5
1	R	53	LEU	21.2
1	O	223	GLY	21.2
1	Q	131	GLY	21.1
1	Q	122	ALA	20.9
1	O	117	ILE	20.9
1	R	143	VAL	20.8
1	P	5	ILE	20.7
1	P	154	LEU	20.7
1	R	111	ALA	20.6
1	Q	305	VAL	20.5
1	O	161	LEU	20.5
1	P	71	ILE	20.4
1	P	168	VAL	20.4
1	Q	270	ILE	20.3
1	R	259	LEU	20.3
1	Q	9	GLY	20.3
1	O	184	ILE	20.3
1	P	11	ILE	20.2
1	P	315	THR	20.2
1	O	168	VAL	20.2
1	P	283	TYR	20.2
1	P	14	ASN	20.1
1	O	217	VAL	20.0
1	P	73	VAL	20.0
1	R	116	VAL	20.0
1	Q	109	LEU	20.0
1	R	318	SER	19.8
1	R	208	THR	19.8
1	O	279	VAL	19.8
1	P	117	ILE	19.7
1	P	99	PHE	19.6

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Mol	Chain	Res	Type	RSRZ
1	O	158	ALA	19.5
1	R	300	ILE	19.5
1	O	203	ILE	19.5
1	O	302	GLY	19.4
1	O	261	ALA	19.4
1	Q	100	THR	19.4
1	P	286	SER	19.3
1	R	242	LEU	19.3
1	R	46	TYR	19.3
1	R	214	VAL	19.1
1	Q	153	CYS	19.0
1	O	129	VAL	19.0
1	R	317	TYR	18.9
1	R	257	ALA	18.9
1	R	81	ASN	18.8
1	R	217	VAL	18.8
1	Q	221	LEU	18.8
1	R	126	ILE	18.8
1	Q	126	ILE	18.7
1	R	42	HIS	18.7
1	Q	160	VAL	18.7
1	R	202	SER	18.6
1	Q	151	THR	18.5
1	P	30	VAL	18.5
1	Q	85	GLY	18.4
1	O	140	ALA	18.3
1	Q	84	TRP	18.3
1	Q	83	ALA	18.3
1	O	118	ILE	18.2
1	P	82	LEU	18.1
1	P	157	PHE	18.1
1	R	235	PRO	18.1
1	R	286	SER	18.0
1	P	109	LEU	18.0
1	O	171	MET	18.0
1	R	310	TRP	17.9
1	R	121	PRO	17.9
1	R	155	ALA	17.9
1	R	252	VAL	17.9
1	Q	28	VAL	17.8
1	Q	128	ILE	17.8
1	Q	256	ASN	17.7

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Mol	Chain	Res	Type	RSRZ
1	P	86	GLU	17.7
1	Q	246	LEU	17.7
1	P	155	ALA	17.6
1	O	143	VAL	17.5
1	O	270	ILE	17.4
1	Q	97	GLY	17.4
1	O	132	VAL	17.4
1	P	242	LEU	17.3
1	R	64	LEU	17.3
1	Q	292	ILE	17.3
1	O	244	ALA	17.3
1	P	53	LEU	17.3
1	Q	171	MET	17.3
1	P	153	CYS	17.3
1	O	79	PRO	17.2
1	Q	298	MET	17.2
1	R	128	ILE	17.1
1	O	156	PRO	17.1
1	P	81	ASN	17.1
1	R	30	VAL	17.0
1	P	113	ALA	17.0
1	O	307	VAL	17.0
1	P	213	ALA	17.0
1	O	230	MET	16.9
1	O	48	SER	16.9
1	Q	297	THR	16.9
1	R	221	LEU	16.9
1	Q	22	ASN	16.8
1	O	226	ASN	16.8
1	Q	6	ASN	16.8
1	O	300	ILE	16.7
1	P	142	HIS	16.7
1	Q	255	VAL	16.6
1	P	211	ALA	16.6
1	P	285	GLY	16.6
1	O	153	CYS	16.6
1	P	310	TRP	16.5
1	P	93	VAL	16.5
1	Q	92	VAL	16.5
1	Q	322	VAL	16.5
1	R	269	GLY	16.5
1	O	199	ALA	16.4

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Mol	Chain	Res	Type	RSRZ
1	R	139	LYS	16.4
1	Q	262	ALA	16.4
1	P	322	VAL	16.3
1	P	221	LEU	16.3
1	O	78	ASP	16.3
1	R	156	PRO	16.3
1	Q	238	SER	16.3
1	R	47	ASP	16.3
1	O	125	ASP	16.2
1	R	223	GLY	16.2
1	R	40	LEU	16.2
1	R	119	SER	16.2
1	P	298	MET	16.2
1	O	102	ARG	16.2
1	Q	333	LEU	16.2
1	O	228	MET	16.2
1	Q	120	ALA	16.2
1	Q	143	VAL	16.1
1	Q	20	LEU	16.1
1	Q	140	ALA	16.1
1	P	222	LYS	16.1
1	Q	152	ASN	16.0
1	Q	244	ALA	16.0
1	O	301	ASP	16.0
1	O	81	ASN	16.0
1	R	226	ASN	16.0
1	O	202	SER	15.9
1	Q	62	ASN	15.9
1	O	109	LEU	15.9
1	R	110	GLU	15.9
1	O	243	VAL	15.8
1	Q	222	LYS	15.8
1	Q	242	LEU	15.8
1	R	168	VAL	15.7
1	Q	154	LEU	15.7
1	Q	167	ILE	15.7
1	O	154	LEU	15.7
1	Q	23	PRO	15.6
1	R	48	SER	15.6
1	Q	71	ILE	15.6
1	R	84	TRP	15.6
1	Q	29	ALA	15.5

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Mol	Chain	Res	Type	RSRZ
1	Q	142	HIS	15.5
1	P	48	SER	15.4
1	R	250	VAL	15.4
1	Q	274	SER	15.4
1	R	311	TYR	15.4
1	Q	157	PHE	15.4
1	O	219	PRO	15.4
1	P	279	VAL	15.3
1	R	144	ILE	15.3
1	P	116	VAL	15.3
1	Q	156	PRO	15.3
1	R	160	VAL	15.3
1	R	307	VAL	15.3
1	P	120	ALA	15.2
1	R	83	ALA	15.2
1	R	147	ALA	15.2
1	P	100	THR	15.2
1	O	144	ILE	15.2
1	R	93	VAL	15.2
1	P	277	PRO	15.1
1	P	237	VAL	15.1
1	P	146	ASN	15.1
1	P	307	VAL	15.1
1	R	262	ALA	15.1
1	R	14	ASN	15.1
1	Q	267	LEU	15.1
1	R	211	ALA	15.1
1	Q	91	ILE	15.0
1	O	198	ALA	15.0
1	Q	288	VAL	15.0
1	Q	220	GLU	15.0
1	R	273	TYR	14.9
1	P	305	VAL	14.9
1	P	37	ALA	14.9
1	R	171	MET	14.9
1	R	153	CYS	14.9
1	O	251	THR	14.9
1	O	262	ALA	14.8
1	Q	309	SER	14.8
1	O	267	LEU	14.8
1	Q	72	ILE	14.8
1	Q	34	THR	14.7

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Mol	Chain	Res	Type	RSRZ
1	O	113	ALA	14.7
1	R	8	PHE	14.7
1	Q	330	SER	14.7
1	R	49	VAL	14.7
1	P	287	THR	14.7
1	P	78	ASP	14.6
1	Q	121	PRO	14.6
1	P	280	SER	14.6
1	P	160	VAL	14.6
1	R	6	ASN	14.6
1	O	240	VAL	14.6
1	Q	214	VAL	14.6
1	P	301	ASP	14.6
1	Q	187	LEU	14.6
1	Q	243	VAL	14.6
1	P	143	VAL	14.5
1	Q	108	HIS	14.5
1	P	171	MET	14.5
1	Q	27	VAL	14.5
1	P	258	ALA	14.5
1	R	80	GLU	14.5
1	O	259	LEU	14.4
1	O	304	MET	14.4
1	P	57	VAL	14.4
1	P	300	ILE	14.4
1	R	149	CYS	14.4
1	Q	263	ALA	14.4
1	P	276	GLU	14.4
1	Q	32	ASP	14.4
1	Q	251	THR	14.4
1	P	8	PHE	14.4
1	P	127	THR	14.4
1	P	218	LEU	14.4
1	R	73	VAL	14.3
1	P	40	LEU	14.3
1	R	122	ALA	14.3
1	Q	165	PHE	14.3
1	O	148	SER	14.3
1	R	131	GLY	14.3
1	R	213	ALA	14.3
1	O	89	VAL	14.3
1	Q	67	ASN	14.3

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Mol	Chain	Res	Type	RSRZ
1	P	129	VAL	14.2
1	Q	307	VAL	14.2
1	O	263	ALA	14.2
1	O	145	SER	14.2
1	Q	290	SER	14.2
1	P	136	LYS	14.2
1	O	116	VAL	14.2
1	P	248	LYS	14.1
1	Q	159	LYS	14.1
1	P	278	LEU	14.1
1	Q	96	THR	14.1
1	P	84	TRP	14.1
1	O	257	ALA	14.1
1	Q	138(A)	PRO	14.0
1	R	321	VAL	14.0
1	P	128	ILE	14.0
1	O	187	LEU	14.0
1	O	269	GLY	14.0
1	O	252	VAL	14.0
1	Q	134	GLN	14.0
1	P	158	ALA	14.0
1	O	214	VAL	14.0
1	P	172	MET	14.0
1	R	140	ALA	14.0
1	P	187	LEU	13.9
1	Q	237	VAL	13.9
1	R	99	PHE	13.9
1	Q	295	LEU	13.9
1	Q	99	PHE	13.9
1	R	295	LEU	13.9
1	Q	68	GLY	13.9
1	R	41	ALA	13.9
1	R	261	ALA	13.9
1	P	141	HIS	13.9
1	O	207	THR	13.8
1	P	299	VAL	13.8
1	P	167	ILE	13.8
1	P	314	GLU	13.8
1	O	100	THR	13.8
1	R	141	HIS	13.8
1	R	44	LEU	13.8
1	R	151	THR	13.7

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Mol	Chain	Res	Type	RSRZ
1	P	232	VAL	13.7
1	Q	141	HIS	13.7
1	R	108	HIS	13.7
1	Q	116	VAL	13.7
1	O	128	ILE	13.7
1	P	126	ILE	13.7
1	P	170	GLY	13.7
1	O	299	VAL	13.6
1	P	207	THR	13.6
1	Q	173	THR	13.6
1	Q	104	ASP	13.6
1	Q	310	TRP	13.6
1	R	290	SER	13.6
1	O	36	ASP	13.5
1	R	31	ASN	13.5
1	Q	15	VAL	13.5
1	Q	327	TYR	13.5
1	P	259	LEU	13.4
1	Q	204	ILE	13.4
1	P	152	ASN	13.3
1	R	137	TYR	13.3
1	Q	63	ASN	13.3
1	O	213	ALA	13.3
1	P	79	PRO	13.3
1	O	333	LEU	13.3
1	P	311	TYR	13.3
1	R	32	ASP	13.3
1	O	155	ALA	13.3
1	R	59	VAL	13.2
1	O	18	ALA	13.2
1	R	167	ILE	13.2
1	P	156	PRO	13.2
1	R	163	GLU	13.2
1	Q	190	HIS	13.2
1	Q	257	ALA	13.2
1	R	216	LEU	13.2
1	O	11	ILE	13.2
1	R	161	LEU	13.2
1	Q	320	ARG	13.2
1	R	218	LEU	13.1
1	O	84	TRP	13.1
1	R	17	ARG	13.1

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Mol	Chain	Res	Type	RSRZ
1	Q	129	VAL	13.1
1	R	169	ARG	13.1
1	O	205	PRO	13.1
1	R	244	ALA	13.1
1	R	142	HIS	13.1
1	Q	39	THR	13.1
1	Q	60	ASN	13.1
1	R	165	PHE	13.1
1	P	193	LEU	13.0
1	Q	218	LEU	13.0
1	R	260	LYS	13.0
1	R	120	ALA	13.0
1	Q	155	ALA	13.0
1	P	145	SER	13.0
1	Q	93	VAL	13.0
1	P	31	ASN	13.0
1	Q	168	VAL	12.9
1	R	322	VAL	12.9
1	R	78	ASP	12.9
1	Q	318	SER	12.9
1	Q	61	GLY	12.9
1	Q	223	GLY	12.9
1	R	92	VAL	12.9
1	Q	16	PHE	12.8
1	O	19	ALA	12.8
1	Q	207	THR	12.8
1	P	209	GLY	12.8
1	Q	26	GLU	12.8
1	Q	123	ASN	12.8
1	Q	132	VAL	12.8
1	P	83	ALA	12.8
1	O	255	VAL	12.8
1	R	204	ILE	12.8
1	O	225	LEU	12.8
1	O	80	GLU	12.7
1	R	148	SER	12.7
1	Q	209	GLY	12.7
1	P	16	PHE	12.7
1	Q	24	ASP	12.7
1	P	196	ALA	12.7
1	Q	210	ALA	12.7
1	P	306	LYS	12.7

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Mol	Chain	Res	Type	RSRZ
1	Q	59	VAL	12.7
1	R	304	MET	12.6
1	O	87	ILE	12.6
1	R	39	THR	12.6
1	O	188	PRO	12.6
1	P	225	LEU	12.5
1	Q	212	LYS	12.5
1	Q	321	VAL	12.5
1	Q	5	ILE	12.5
1	O	193	LEU	12.5
1	O	196	ALA	12.5
1	Q	122(A)	LYS	12.5
1	P	250	VAL	12.5
1	O	99	PHE	12.5
1	R	91	ILE	12.4
1	P	295	LEU	12.4
1	R	16	PHE	12.4
1	R	85	GLY	12.4
1	P	7	GLY	12.4
1	P	291	THR	12.4
1	O	139	LYS	12.4
1	O	310	TRP	12.4
1	Q	240	VAL	12.4
1	R	133	ASN	12.4
1	O	246	LEU	12.4
1	R	178	TYR	12.4
1	R	13	ARG	12.3
1	R	246	LEU	12.3
1	P	292	ILE	12.3
1	P	308	VAL	12.3
1	Q	8	PHE	12.3
1	P	318	SER	12.3
1	R	284	ASN	12.3
1	R	270	ILE	12.3
1	R	146	ASN	12.2
1	O	39	THR	12.2
1	O	284	ASN	12.2
1	R	249	GLU	12.2
1	P	214	VAL	12.2
1	O	224	LYS	12.2
1	P	111	ALA	12.2
1	Q	14	ASN	12.2

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Mol	Chain	Res	Type	RSRZ
1	P	162	HIS	12.2
1	Q	136	LYS	12.2
1	Q	299	VAL	12.2
1	R	239	VAL	12.2
1	P	185	LEU	12.1
1	P	198	ALA	12.1
1	Q	249	GLU	12.1
1	R	37	ALA	12.1
1	P	282	ASP	12.1
1	P	293	ASP	12.0
1	P	316	GLY	12.0
1	P	32	ASP	12.0
1	R	125	ASP	12.0
1	R	227	GLY	12.0
1	O	138(A)	PRO	12.0
1	R	62	ASN	12.0
1	Q	282	ASP	12.0
1	O	82	LEU	11.9
1	P	122(A)	LYS	11.9
1	Q	7	GLY	11.9
1	P	50	HIS	11.9
1	Q	314	GLU	11.9
1	P	324	LEU	11.9
1	Q	10	ARG	11.8
1	R	150	THR	11.8
1	Q	188	PRO	11.8
1	Q	82	LEU	11.8
1	P	321	VAL	11.8
1	R	9	GLY	11.8
1	O	329	ALA	11.7
1	Q	289	SER	11.7
1	R	251	THR	11.7
1	O	273	TYR	11.7
1	P	175	VAL	11.7
1	P	219	PRO	11.7
1	Q	170	GLY	11.7
1	R	225	LEU	11.7
1	O	55	ALA	11.7
1	R	100	THR	11.6
1	O	37	ALA	11.6
1	O	186	ASP	11.6
1	O	204	ILE	11.6

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Mol	Chain	Res	Type	RSRZ
1	O	12	GLY	11.6
1	Q	324	LEU	11.6
1	P	290	SER	11.5
1	O	229	ALA	11.5
1	P	36	ASP	11.5
1	R	185	LEU	11.5
1	Q	58	SER	11.5
1	P	297	THR	11.5
1	P	243	VAL	11.5
1	P	75	ALA	11.5
1	R	200	ALA	11.5
1	O	283	TYR	11.5
1	O	218	LEU	11.5
1	P	42	HIS	11.5
1	P	309	SER	11.5
1	P	312	ASP	11.5
1	P	252	VAL	11.4
1	R	145	SER	11.4
1	P	289	SER	11.4
1	O	254	GLU	11.4
1	R	230	MET	11.4
1	P	208	THR	11.4
1	Q	227	GLY	11.3
1	Q	217	VAL	11.3
1	Q	224	LYS	11.3
1	O	108	HIS	11.3
1	Q	113	ALA	11.3
1	Q	162	HIS	11.3
1	O	130	MET	11.3
1	O	141	HIS	11.3
1	R	288	VAL	11.2
1	R	253	GLU	11.2
1	Q	219	PRO	11.2
1	O	183	ARG	11.2
1	O	297	THR	11.2
1	Q	18	ALA	11.2
1	P	288	VAL	11.2
1	Q	273	TYR	11.2
1	O	54	ASP	11.2
1	Q	98	ARG	11.2
1	R	18	ALA	11.2
1	O	73	VAL	11.2

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Mol	Chain	Res	Type	RSRZ
1	Q	86	GLU	11.2
1	O	107	LYS	11.2
1	R	301	ASP	11.2
1	R	237	VAL	11.2
1	O	7	GLY	11.2
1	Q	161	LEU	11.2
1	Q	31	ASN	11.1
1	Q	78	ASP	11.1
1	R	52	ARG	11.1
1	R	320	ARG	11.1
1	O	44	LEU	11.1
1	O	216	LEU	11.1
1	R	154	LEU	11.1
1	P	274	SER	11.1
1	Q	150	THR	11.1
1	Q	144	ILE	11.1
1	P	105	ALA	11.1
1	R	274	SER	11.1
1	P	15	VAL	11.0
1	P	132	VAL	11.0
1	P	103	GLU	11.0
1	O	68	GLY	11.0
1	R	243	VAL	11.0
1	R	184	ILE	11.0
1	O	33	LEU	11.0
1	Q	199	ALA	11.0
1	O	27	VAL	11.0
1	R	207	THR	11.0
1	R	294	ALA	11.0
1	Q	48	SER	11.0
1	P	178	TYR	10.9
1	Q	328	ILE	10.9
1	P	260	LYS	10.9
1	O	57	VAL	10.9
1	R	240	VAL	10.9
1	R	255	VAL	10.9
1	O	67	ASN	10.9
1	O	120	ALA	10.9
1	O	294	ALA	10.9
1	R	94	GLU	10.9
1	R	38	ASN	10.9
1	R	298	MET	10.9

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Mol	Chain	Res	Type	RSRZ
1	O	327	TYR	10.9
1	R	122(A)	LYS	10.9
1	P	273	TYR	10.8
1	O	220	GLU	10.8
1	P	6	ASN	10.8
1	O	138	ASP	10.8
1	O	296	SER	10.8
1	Q	316	GLY	10.8
1	O	69	LYS	10.8
1	O	163	GLU	10.8
1	Q	65	VAL	10.8
1	Q	110	GLU	10.7
1	Q	130	MET	10.7
1	O	328	ILE	10.7
1	Q	69	LYS	10.7
1	R	234	THR	10.7
1	R	254	GLU	10.7
1	O	295	LEU	10.7
1	Q	193	LEU	10.7
1	Q	286	SER	10.7
1	P	44	LEU	10.7
1	R	287	THR	10.7
1	O	258	ALA	10.7
1	P	203	ILE	10.6
1	Q	41	ALA	10.6
1	Q	4	GLY	10.6
1	P	118	ILE	10.6
1	Q	174	THR	10.6
1	O	86	GLU	10.6
1	Q	2	LYS	10.6
1	R	7	GLY	10.6
1	R	279	VAL	10.6
1	Q	228	MET	10.5
1	P	284	ASN	10.5
1	Q	216	LEU	10.5
1	O	91	ILE	10.5
1	R	95	SER	10.5
1	R	82	LEU	10.5
1	Q	232	VAL	10.5
1	R	247	GLU	10.5
1	O	288	VAL	10.5
1	Q	105	ALA	10.5

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Mol	Chain	Res	Type	RSRZ
1	Q	81	ASN	10.4
1	Q	133	ASN	10.4
1	Q	163	GLU	10.4
1	R	186	ASP	10.4
1	P	217	VAL	10.4
1	Q	135	ASP	10.4
1	P	304	MET	10.4
1	Q	215	ALA	10.4
1	R	3	VAL	10.4
1	R	328	ILE	10.4
1	Q	332	GLY	10.4
1	Q	329	ALA	10.4
1	R	175	VAL	10.4
1	P	247	GLU	10.4
1	P	119	SER	10.4
1	R	224	LYS	10.4
1	Q	197	ARG	10.4
1	Q	175	VAL	10.4
1	P	263	ALA	10.3
1	Q	208	THR	10.3
1	R	34	THR	10.3
1	Q	254	GLU	10.3
1	R	206	THR	10.3
1	P	17	ARG	10.3
1	P	124	GLU	10.3
1	P	319	HIS	10.3
1	Q	325	ALA	10.3
1	P	39	THR	10.3
1	P	74	LYS	10.3
1	O	305	VAL	10.3
1	Q	184	ILE	10.3
1	O	110	GLU	10.3
1	P	281	ARG	10.3
1	Q	3	VAL	10.3
1	Q	70	GLU	10.3
1	O	119	SER	10.2
1	R	115	LYS	10.2
1	O	212	LYS	10.2
1	Q	239	VAL	10.2
1	R	229	ALA	10.2
1	R	103	GLU	10.2
1	P	234	THR	10.2

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Mol	Chain	Res	Type	RSRZ
1	Q	203	ILE	10.2
1	P	294	ALA	10.2
1	O	142	HIS	10.2
1	R	190	HIS	10.2
1	R	209	GLY	10.2
1	Q	77	ARG	10.1
1	R	179	THR	10.1
1	O	318	SER	10.1
1	O	311	TYR	10.1
1	R	296	SER	10.1
1	Q	185	LEU	10.1
1	Q	21	LYS	10.1
1	P	133	ASN	10.1
1	Q	103	GLU	10.1
1	P	108	HIS	10.1
1	O	324	LEU	10.0
1	P	241	ASP	10.0
1	Q	164	GLN	10.0
1	O	111	ALA	10.0
1	Q	53	LEU	10.0
1	R	130	MET	10.0
1	O	94	GLU	10.0
1	O	190	HIS	10.0
1	P	165	PHE	10.0
1	O	210	ALA	10.0
1	P	216	LEU	10.0
1	O	206	THR	10.0
1	R	57	VAL	10.0
1	Q	127	THR	10.0
1	R	241	ASP	10.0
1	O	166	GLY	10.0
1	R	292	ILE	10.0
1	Q	271	LEU	9.9
1	O	15	VAL	9.9
1	Q	229	ALA	9.9
1	Q	115	LYS	9.9
1	O	51	GLY	9.9
1	O	93	VAL	9.9
1	R	152	ASN	9.9
1	R	187	LEU	9.9
1	P	101	LYS	9.9
1	R	76	GLU	9.9

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Mol	Chain	Res	Type	RSRZ
1	O	164	GLN	9.8
1	O	298	MET	9.8
1	R	291	THR	9.8
1	P	182	GLN	9.8
1	O	321	VAL	9.8
1	Q	261	ALA	9.8
1	Q	269	GLY	9.8
1	Q	283	TYR	9.8
1	O	25	ILE	9.8
1	Q	172	MET	9.8
1	O	222	LYS	9.7
1	O	95	SER	9.7
1	Q	319	HIS	9.7
1	O	90	ASP	9.7
1	O	293	ASP	9.7
1	R	188	PRO	9.7
1	R	297	THR	9.6
1	O	0	ALA	9.6
1	O	22	ASN	9.6
1	R	173	THR	9.6
1	O	16	PHE	9.6
1	R	324	LEU	9.6
1	P	77	ARG	9.5
1	O	114	LYS	9.5
1	P	64	LEU	9.5
1	R	159	LYS	9.5
1	P	80	GLU	9.5
1	O	167	ILE	9.5
1	O	197	ARG	9.5
1	O	227	GLY	9.5
1	O	256	ASN	9.5
1	P	96	THR	9.5
1	P	255	VAL	9.5
1	R	319	HIS	9.5
1	Q	64	LEU	9.5
1	R	33	LEU	9.5
1	O	162	HIS	9.5
1	Q	89	VAL	9.5
1	P	13	ARG	9.4
1	O	65	VAL	9.4
1	O	308	VAL	9.4
1	P	210	ALA	9.4

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Mol	Chain	Res	Type	RSRZ
1	Q	42	HIS	9.4
1	P	235	PRO	9.4
1	O	47	ASP	9.4
1	O	137	TYR	9.4
1	O	247	GLU	9.4
1	Q	198	ALA	9.4
1	R	50	HIS	9.4
1	O	178	TYR	9.3
1	R	61	GLY	9.3
1	O	146	ASN	9.3
1	P	58	SER	9.3
1	P	246	LEU	9.3
1	P	45	LYS	9.3
1	Q	90	ASP	9.3
1	O	211	ALA	9.3
1	P	173	THR	9.3
1	Q	106	ALA	9.3
1	R	138	ASP	9.3
1	Q	101	LYS	9.3
1	R	309	SER	9.3
1	R	256	ASN	9.3
1	Q	266	GLU	9.3
1	Q	38	ASN	9.3
1	P	104	ASP	9.2
1	O	104	ASP	9.2
1	Q	40	LEU	9.2
1	O	170	GLY	9.2
1	R	51	GLY	9.2
1	R	283	TYR	9.2
1	P	107	LYS	9.2
1	Q	313	ASN	9.2
1	O	3	VAL	9.2
1	O	306	LYS	9.2
1	P	191	LYS	9.2
1	P	122	ALA	9.2
1	O	64	LEU	9.2
1	P	199	ALA	9.2
1	Q	258	ALA	9.2
1	R	215	ALA	9.2
1	O	88	GLY	9.2
1	P	131	GLY	9.2
1	O	253	GLU	9.2

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Mol	Chain	Res	Type	RSRZ
1	R	222	LYS	9.2
1	R	245	GLU	9.2
1	P	204	ILE	9.2
1	O	289	SER	9.2
1	O	136	LYS	9.2
1	Q	46	TYR	9.2
1	O	5	ILE	9.2
1	P	236	ASN	9.1
1	O	29	ALA	9.1
1	O	75	ALA	9.1
1	Q	57	VAL	9.1
1	P	46	TYR	9.1
1	R	79	PRO	9.1
1	R	74	LYS	9.1
1	Q	137	TYR	9.1
1	Q	118	ILE	9.1
1	R	308	VAL	9.1
1	O	8	PHE	9.1
1	P	63	ASN	9.1
1	O	274	SER	9.1
1	O	2	LYS	9.1
1	O	30	VAL	9.0
1	O	180	ASN	9.0
1	Q	79	PRO	9.0
1	P	98	ARG	9.0
1	R	266	GLU	9.0
1	R	172	MET	9.0
1	P	33	LEU	9.0
1	P	94	GLU	9.0
1	R	114	LYS	9.0
1	P	176	HIS	9.0
1	O	249	GLU	9.0
1	O	6	ASN	9.0
1	O	60	ASN	9.0
1	R	98	ARG	9.0
1	R	162	HIS	9.0
1	Q	235	PRO	9.0
1	O	59	VAL	9.0
1	P	125	ASP	9.0
1	P	184	ILE	8.9
1	R	109	LEU	8.9
1	O	278	LEU	8.9

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Mol	Chain	Res	Type	RSRZ
1	O	287	THR	8.9
1	Q	125	ASP	8.9
1	O	42	HIS	8.9
1	Q	50	HIS	8.9
1	Q	54	ASP	8.9
1	Q	326	ALA	8.9
1	Q	206	THR	8.8
1	Q	138	ASP	8.8
1	Q	241	ASP	8.8
1	Q	94	GLU	8.8
1	Q	272	ALA	8.8
1	O	49	VAL	8.8
1	O	250	VAL	8.8
1	R	174	THR	8.8
1	P	228	MET	8.8
1	R	107	LYS	8.8
1	O	272	ALA	8.8
1	Q	279	VAL	8.8
1	P	18	ALA	8.8
1	R	136	LYS	8.8
1	Q	259	LEU	8.8
1	R	10	ARG	8.8
1	O	237	VAL	8.8
1	P	238	SER	8.8
1	Q	291	THR	8.7
1	Q	245	GLU	8.7
1	O	174	THR	8.7
1	Q	179	THR	8.7
1	R	166	GLY	8.7
1	R	170	GLY	8.7
1	O	149	CYS	8.7
1	P	257	ALA	8.7
1	O	248	LYS	8.7
1	R	314	GLU	8.7
1	P	121	PRO	8.7
1	O	322	VAL	8.7
1	Q	301	ASP	8.7
1	R	236	ASN	8.6
1	O	271	LEU	8.6
1	R	203	ILE	8.6
1	O	14	ASN	8.6
1	R	123	ASN	8.6

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Mol	Chain	Res	Type	RSRZ
1	O	61	GLY	8.6
1	Q	25	ILE	8.6
1	O	147	ALA	8.6
1	O	290	SER	8.6
1	R	263	ALA	8.6
1	O	92	VAL	8.6
1	P	188	PRO	8.5
1	Q	253	GLU	8.5
1	P	212	LYS	8.5
1	R	177	SER	8.5
1	P	10	ARG	8.5
1	P	200	ALA	8.5
1	Q	304	MET	8.5
1	R	45	LYS	8.5
1	O	131	GLY	8.5
1	O	316	GLY	8.5
1	P	190	HIS	8.4
1	Q	200	ALA	8.4
1	R	210	ALA	8.4
1	O	9	GLY	8.4
1	O	17	ARG	8.4
1	O	280	SER	8.4
1	Q	95	SER	8.4
1	O	72	ILE	8.4
1	O	233	PRO	8.4
1	Q	158	ALA	8.4
1	P	224	LYS	8.4
1	O	266	GLU	8.4
1	O	41	ALA	8.4
1	P	244	ALA	8.4
1	R	264	GLU	8.3
1	O	112	GLY	8.3
1	O	40	LEU	8.3
1	P	159	LYS	8.3
1	Q	236	ASN	8.3
1	R	183	ARG	8.3
1	O	238	SER	8.3
1	O	173	THR	8.3
1	Q	284	ASN	8.3
1	R	134	GLN	8.3
1	R	198	ALA	8.2
1	O	264	GLU	8.2

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Mol	Chain	Res	Type	RSRZ
1	Q	119	SER	8.2
1	O	1	VAL	8.2
1	P	151	THR	8.2
1	Q	287	THR	8.2
1	Q	186	ASP	8.2
1	P	169	ARG	8.2
1	Q	139	LYS	8.2
1	R	293	ASP	8.2
1	P	245	GLU	8.2
1	Q	280	SER	8.2
1	Q	107	LYS	8.2
1	R	313	ASN	8.1
1	R	101	LYS	8.1
1	O	241	ASP	8.1
1	P	179	THR	8.1
1	Q	323	ASP	8.1
1	O	122	ALA	8.1
1	Q	36	ASP	8.1
1	R	135	ASP	8.1
1	R	113	ALA	8.1
1	Q	112	GLY	8.1
1	O	315	THR	8.1
1	Q	45	LYS	8.1
1	P	166	GLY	8.1
1	R	315	THR	8.1
1	R	129	VAL	8.0
1	P	194	ARG	8.0
1	Q	306	LYS	8.0
1	R	282	ASP	8.0
1	O	201	GLU	8.0
1	P	9	GLY	8.0
1	R	97	GLY	8.0
1	O	239	VAL	8.0
1	Q	312	ASP	8.0
1	R	278	LEU	8.0
1	O	96	THR	7.9
1	O	194	ARG	7.9
1	Q	176	HIS	7.9
1	O	172	MET	7.9
1	Q	52	ARG	7.9
1	O	312	ASP	7.9
1	O	24	ASP	7.9

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Mol	Chain	Res	Type	RSRZ
1	R	96	THR	7.9
1	R	196	ALA	7.8
1	P	97	GLY	7.8
1	P	148	SER	7.8
1	Q	66	VAL	7.8
1	P	174	THR	7.8
1	P	296	SER	7.8
1	O	23	PRO	7.8
1	R	77	ARG	7.8
1	Q	180	ASN	7.8
1	O	176	HIS	7.8
1	P	164	GLN	7.7
1	P	229	ALA	7.7
1	O	77	ARG	7.7
1	Q	213	ALA	7.7
1	O	31	ASN	7.7
1	Q	56	GLU	7.7
1	O	159	LYS	7.7
1	P	51	GLY	7.7
1	Q	87	ILE	7.7
1	O	133	ASN	7.7
1	R	285	GLY	7.7
1	O	317	TYR	7.7
1	O	66	VAL	7.7
1	P	43	LEU	7.7
1	P	149	CYS	7.6
1	Q	102	ARG	7.6
1	P	220	GLU	7.6
1	R	232	VAL	7.6
1	R	105	ALA	7.6
1	O	232	VAL	7.6
1	O	303	LYS	7.6
1	O	71	ILE	7.6
1	P	38	ASN	7.6
1	P	272	ALA	7.6
1	O	282	ASP	7.6
1	Q	296	SER	7.6
1	O	234	THR	7.6
1	O	177	SER	7.5
1	Q	37	ALA	7.5
1	P	262	ALA	7.5
1	R	106	ALA	7.5

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Mol	Chain	Res	Type	RSRZ
1	O	101	LYS	7.5
1	O	192	ASP	7.5
1	R	192	ASP	7.5
1	P	256	ASN	7.5
1	Q	281	ARG	7.5
1	R	193	LEU	7.5
1	P	192	ASP	7.5
1	Q	225	LEU	7.4
1	R	271	LEU	7.4
1	R	132	VAL	7.4
1	O	50	HIS	7.4
1	Q	169	ARG	7.4
1	O	123	ASN	7.4
1	O	46	TYR	7.4
1	P	102	ARG	7.4
1	P	62	ASN	7.4
1	O	34	THR	7.4
1	O	20	LEU	7.4
1	Q	43	LEU	7.4
1	R	316	GLY	7.4
1	O	319	HIS	7.4
1	R	267	LEU	7.4
1	R	248	LYS	7.3
1	O	76	GLU	7.3
1	O	121	PRO	7.3
1	O	122(A)	LYS	7.3
1	R	277	PRO	7.3
1	O	200	ALA	7.3
1	O	28	VAL	7.2
1	O	175	VAL	7.2
1	P	249	GLU	7.2
1	O	331	LYS	7.2
1	O	325	ALA	7.2
1	Q	293	ASP	7.2
1	O	195	ARG	7.2
1	O	332	GLY	7.2
1	O	53	LEU	7.2
1	P	275	GLU	7.2
1	R	104	ASP	7.2
1	R	275	GLU	7.2
1	R	220	GLU	7.2
1	O	97	GLY	7.1

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Mol	Chain	Res	Type	RSRZ
1	O	236	ASN	7.1
1	Q	44	LEU	7.1
1	Q	51	GLY	7.1
1	Q	230	MET	7.1
1	O	245	GLU	7.1
1	P	233	PRO	7.1
1	Q	124	GLU	7.1
1	O	169	ARG	7.1
1	O	135	ASP	7.0
1	Q	234	THR	7.0
1	R	199	ALA	7.0
1	O	231	ARG	7.0
1	P	251	THR	7.0
1	O	265	GLY	7.0
1	Q	147	ALA	7.0
1	Q	205	PRO	7.0
1	O	286	SER	7.0
1	P	95	SER	7.0
1	O	208	THR	6.9
1	O	124	GLU	6.9
1	P	130	MET	6.9
1	Q	211	ALA	6.9
1	O	62	ASN	6.9
1	Q	17	ARG	6.9
1	O	309	SER	6.8
1	P	150	THR	6.8
1	Q	231	ARG	6.8
1	R	89	VAL	6.8
1	P	47	ASP	6.8
1	O	326	ALA	6.7
1	Q	49	VAL	6.7
1	Q	47	ASP	6.7
1	R	228	MET	6.7
1	Q	277	PRO	6.7
1	O	281	ARG	6.7
1	R	268	LYS	6.7
1	R	182	GLN	6.7
1	Q	177	SER	6.7
1	Q	285	GLY	6.7
1	Q	192	ASP	6.7
1	P	313	ASN	6.7
1	O	179	THR	6.6

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Mol	Chain	Res	Type	RSRZ
1	O	268	LYS	6.6
1	Q	278	LEU	6.6
1	R	306	LYS	6.6
1	P	76	GLU	6.6
1	O	10	ARG	6.6
1	R	180	ASN	6.6
1	P	177	SER	6.6
1	O	277	PRO	6.6
1	R	233	PRO	6.6
1	P	106	ALA	6.6
1	Q	196	ALA	6.6
1	P	253	GLU	6.5
1	Q	146	ASN	6.5
1	P	181	ASP	6.5
1	Q	191	LYS	6.5
1	R	325	ALA	6.5
1	P	206	THR	6.5
1	Q	276	GLU	6.5
1	O	43	LEU	6.5
1	P	180	ASN	6.5
1	Q	166	GLY	6.5
1	P	163	GLU	6.5
1	O	115	LYS	6.4
1	Q	303	LYS	6.4
1	P	320	ARG	6.4
1	P	123	ASN	6.4
1	O	85	GLY	6.4
1	R	205	PRO	6.4
1	R	164	GLN	6.4
1	R	197	ARG	6.4
1	Q	80	GLU	6.4
1	R	323	ASP	6.3
1	P	197	ARG	6.3
1	O	4	GLY	6.3
1	O	209	GLY	6.3
1	R	102	ARG	6.3
1	R	280	SER	6.3
1	O	74	LYS	6.3
1	O	291	THR	6.3
1	Q	55	ALA	6.3
1	O	182	GLN	6.3
1	R	238	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	O	63	ASN	6.2
1	O	58	SER	6.2
1	O	103	GLU	6.2
1	P	34	THR	6.2
1	R	194	ARG	6.2
1	O	235	PRO	6.2
1	O	323	ASP	6.2
1	Q	233	PRO	6.2
1	Q	178	TYR	6.2
1	P	303	LYS	6.2
1	R	212	LYS	6.2
1	O	134	GLN	6.2
1	O	313	ASN	6.1
1	P	254	GLU	6.1
1	P	110	GLU	6.1
1	O	38	ASN	6.1
1	R	195	ARG	6.1
1	P	183	ARG	6.1
1	R	138(A)	PRO	6.1
1	R	181	ASP	6.0
1	R	281	ARG	6.0
1	R	219	PRO	6.0
1	P	267	LEU	6.0
1	Q	76	GLU	6.0
1	R	201	GLU	6.0
1	O	152	ASN	6.0
1	Q	226	ASN	6.0
1	P	230	MET	6.0
1	P	227	GLY	5.9
1	O	181	ASP	5.9
1	Q	74	LYS	5.9
1	P	202	SER	5.9
1	O	151	THR	5.9
1	P	231	ARG	5.9
1	O	320	ARG	5.9
1	Q	202	SER	5.8
1	O	26	GLU	5.8
1	Q	248	LYS	5.8
1	O	32	ASP	5.8
1	O	52	ARG	5.7
1	Q	195	ARG	5.7
1	O	260	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	Q	247	GLU	5.7
1	P	226	ASN	5.7
1	R	276	GLU	5.7
1	P	52	ARG	5.6
1	O	150	THR	5.6
1	O	285	GLY	5.6
1	O	13	ARG	5.6
1	Q	183	ARG	5.5
1	Q	331	LYS	5.5
1	R	272	ALA	5.5
1	P	201	GLU	5.4
1	O	98	ARG	5.4
1	Q	265	GLY	5.4
1	O	276	GLU	5.4
1	P	270	ILE	5.3
1	R	124	GLU	5.3
1	Q	13	ARG	5.3
1	Q	275	GLU	5.3
1	P	60	ASN	5.2
1	Q	268	LYS	5.2
1	Q	260	LYS	5.2
1	R	12	GLY	5.2
1	R	112	GLY	5.2
1	R	289	SER	5.2
1	O	21	LYS	5.2
1	R	231	ARG	5.2
1	R	36	ASP	5.1
1	Q	182	GLN	5.1
1	P	205	PRO	5.1
1	Q	114	LYS	5.1
1	Q	201	GLU	5.1
1	R	312	ASP	5.1
1	Q	194	ARG	5.1
1	R	191	LYS	5.0
1	O	56	GLU	5.0
1	P	195	ARG	5.0
1	R	63	ASN	5.0
1	Q	302	GLY	5.0
1	R	176	HIS	4.9
1	Q	315	THR	4.9
1	Q	111	ALA	4.7
1	R	303	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	O	330	SER	4.6
1	R	302	GLY	4.6
1	O	275	GLU	4.6
1	P	186	ASP	4.5
1	O	191	LYS	4.4
1	Q	264	GLU	4.3
1	Q	181	ASP	4.0
1	P	112	GLY	3.9
1	O	45	LYS	3.9
1	O	314	GLU	3.4
1	O	70	GLU	3.0

## 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 ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	P	336	44/44	0.72	-	4,10,12,17	0
2	SO4	P	338	5/5	0.59	-	33,35,39,40	0
2	SO4	R	338	5/5	0.67	-	23,26,33,33	0
3	NAD	Q	336	44/44	1.00	-	2,10,12,13	0
2	SO4	Q	339	5/5	0.84	-	27,28,32,34	0
2	SO4	P	339	5/5	0.98	-	30,31,34,36	0
2	SO4	Q	338	5/5	0.39	-	20,24,26,28	0
2	SO4	R	339	5/5	0.73	-	26,27,32,38	0
2	SO4	O	339	5/5	0.68	-	23,26,35,37	0
3	NAD	R	336	44/44	1.01	-	7,11,16,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	O	336	44/44	0.51	-	5,9,16,19	0
2	SO4	O	338	5/5	0.34	-	17,18,19,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.