



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:11 PM UTC

PDB ID : 2GD1 / pdb_00002gd1
Title : COENZYME-INDUCED CONFORMATIONAL CHANGES IN GLYCER
ALDEHYDE-3-PHOSPHATE DEHYDROGENASE FROM BACILLUS
STEAROTHERMOPHILLUS
Authors : Skarzynski, T.; Wonacott, A.J.
Deposited on : 1989-06-29
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

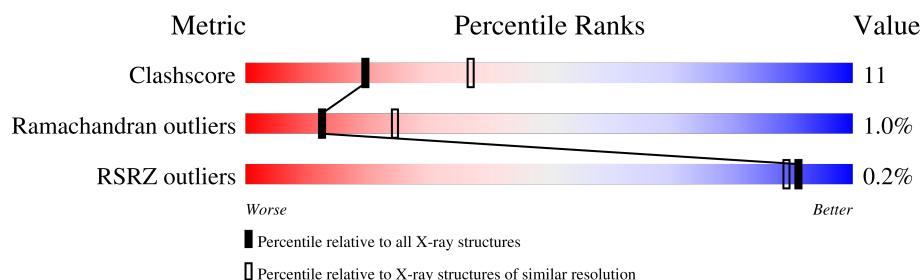
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	334	 57% 34% 9%
1	P	334	 53% 39% 8%
1	Q	334	 58% 35% 7%
1	R	334	 55% 37% 8%

2 Entry composition [i](#)

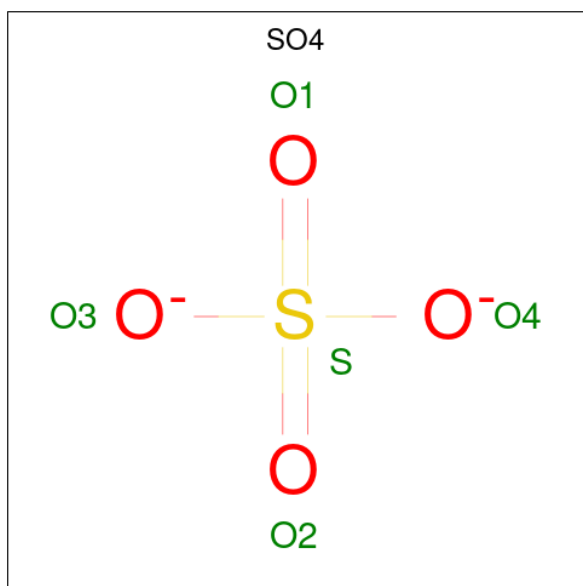
There are 3 unique types of molecules in this entry. The entry contains 10644 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

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 (CCD ID: SO4) (formula: O₄S).



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		

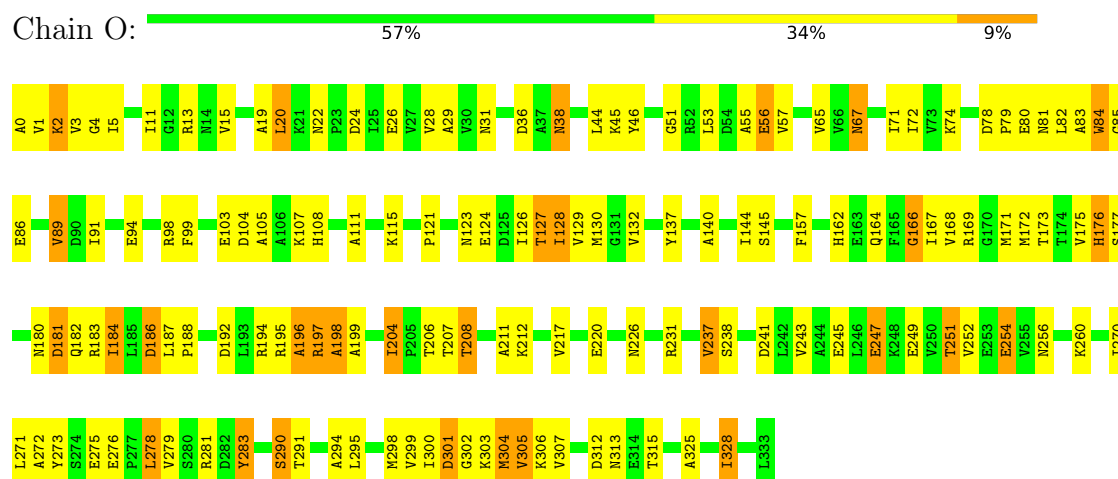
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	114	Total	O	0	0
			114	114		
3	P	127	Total	O	0	0
			127	127		
3	Q	121	Total	O	0	0
			121	121		
3	R	142	Total	O	0	0
			142	142		

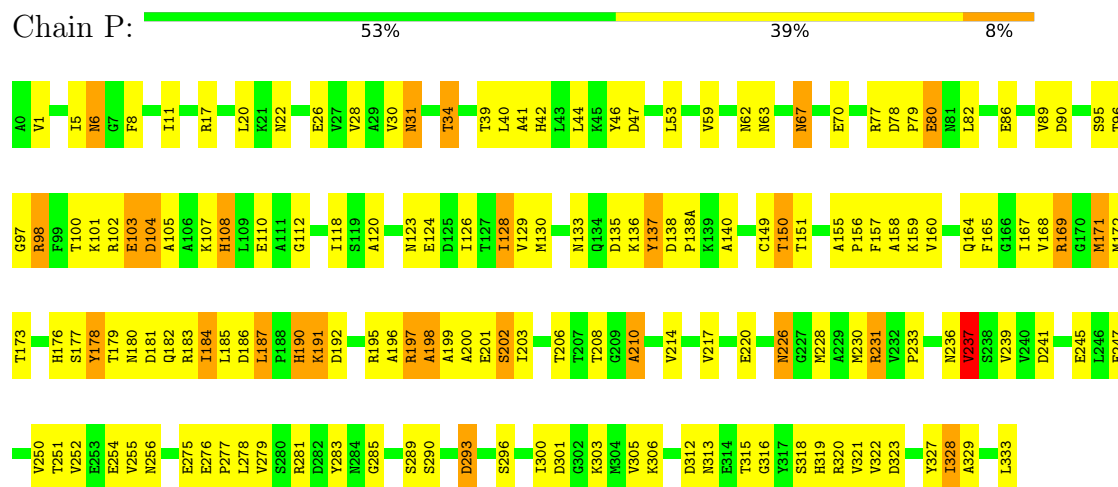
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

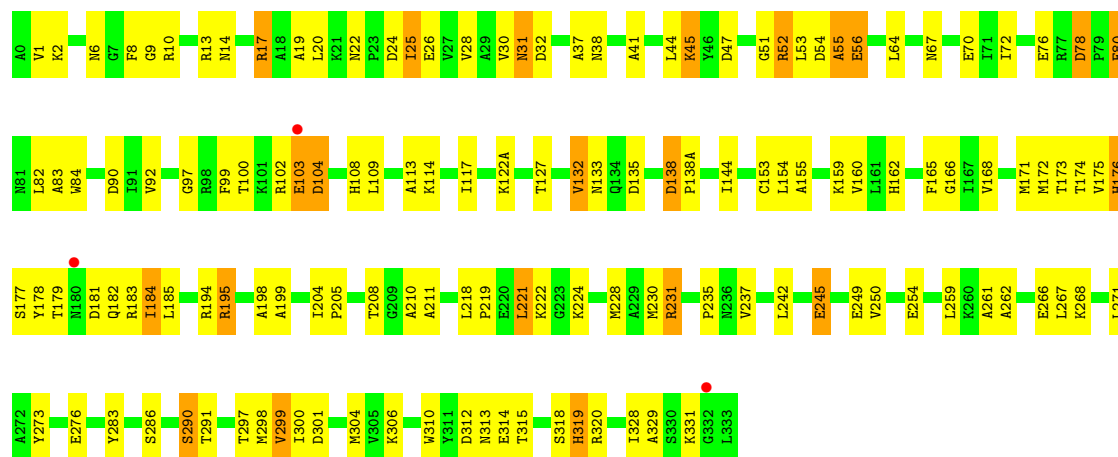


• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



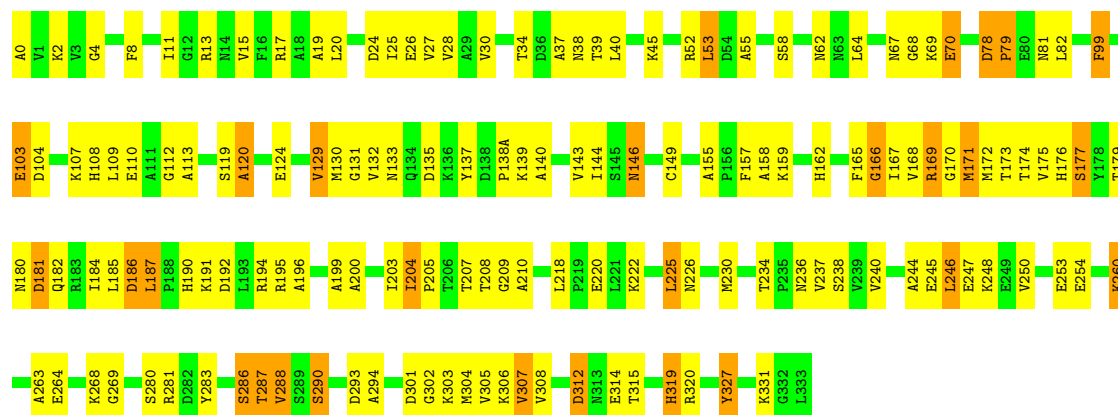
• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain R: 55% 37% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.80Å 129.20Å 83.10Å 90.00° 107.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 80.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 95.2 (80.01-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.50Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10644	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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

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	1.26	1/2561 (0.0%)	2.22	118/3474 (3.4%)
1	P	1.33	2/2561 (0.1%)	2.35	149/3474 (4.3%)
1	Q	1.30	2/2561 (0.1%)	2.30	124/3474 (3.6%)
1	R	1.30	3/2561 (0.1%)	2.38	140/3474 (4.0%)
All	All	1.30	8/10244 (0.1%)	2.31	531/13896 (3.8%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	256	ASN	C-O	6.58	1.31	1.24
1	R	204	ILE	CA-CB	6.00	1.59	1.54
1	P	312	ASP	N-CA	5.41	1.53	1.46
1	R	312	ASP	N-CA	5.19	1.52	1.46
1	Q	231	ARG	C-O	5.16	1.30	1.23
1	O	71	ILE	CA-CB	5.15	1.60	1.54
1	Q	153	CYS	C-N	-5.02	1.26	1.33
1	R	167	ILE	CA-CB	5.01	1.59	1.54

All (531) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	123	ASN	OD1-CG-ND2	13.16	135.76	122.60
1	R	194	ARG	CD-NE-CZ	12.82	142.34	124.40
1	R	204	ILE	N-CA-C	12.81	120.83	108.15
1	R	78	ASP	CA-CB-CG	-12.17	100.43	112.60
1	R	203	ILE	CA-C-N	11.39	135.78	123.25
1	R	203	ILE	C-N-CA	11.39	135.78	123.25
1	P	11	ILE	CA-C-O	-11.12	109.39	121.17
1	Q	102	ARG	CA-C-N	11.01	135.40	120.54
1	Q	102	ARG	C-N-CA	11.01	135.40	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	197	ARG	NE-CZ-NH2	10.89	129.00	119.20
1	R	320	ARG	CD-NE-CZ	10.78	139.49	124.40
1	P	183	ARG	CA-C-N	10.67	134.01	120.56
1	P	183	ARG	C-N-CA	10.67	134.01	120.56
1	R	171	MET	CA-CB-CG	10.26	134.62	114.10
1	Q	13	ARG	CA-C-N	9.97	133.41	120.44
1	Q	13	ARG	C-N-CA	9.97	133.41	120.44
1	O	303	LYS	N-CA-C	9.82	125.39	113.12
1	P	197	ARG	NE-CZ-NH1	9.49	130.99	121.50
1	Q	312	ASP	CA-CB-CG	9.42	122.02	112.60
1	P	281	ARG	CD-NE-CZ	9.37	137.52	124.40
1	O	184	ILE	N-CA-CB	9.05	121.14	110.55
1	Q	103	GLU	CB-CG-CD	8.97	127.85	112.60
1	Q	80	GLU	CB-CG-CD	8.97	127.85	112.60
1	Q	24	ASP	CA-CB-CG	-8.93	103.67	112.60
1	R	187	LEU	O-C-N	8.88	128.13	121.65
1	R	113	ALA	CA-C-O	-8.71	111.76	121.87
1	R	245	GLU	CB-CG-CD	8.68	127.36	112.60
1	Q	319	HIS	CA-CB-CG	-8.56	105.24	113.80
1	Q	22	ASN	CB-CA-C	8.49	119.60	110.17
1	O	130	MET	CB-CA-C	8.48	122.38	110.16
1	P	112	GLY	N-CA-C	8.48	122.66	113.58
1	O	187	LEU	O-C-N	8.48	128.16	121.55
1	Q	38	ASN	CA-CB-CG	-8.43	104.17	112.60
1	O	167	ILE	CA-C-O	-8.42	111.25	120.85
1	Q	183	ARG	CA-C-N	8.38	131.18	120.70
1	Q	183	ARG	C-N-CA	8.38	131.18	120.70
1	R	168	VAL	N-CA-C	-8.37	103.12	110.74
1	R	200	ALA	CA-C-N	8.36	136.38	121.92
1	R	200	ALA	C-N-CA	8.36	136.38	121.92
1	P	191	LYS	CA-CB-CG	8.34	130.79	114.10
1	Q	38	ASN	CA-C-N	8.29	132.06	120.29
1	Q	38	ASN	C-N-CA	8.29	132.06	120.29
1	R	140	ALA	N-CA-C	8.28	123.57	113.38
1	O	177	SER	CA-CB-OG	-8.27	94.56	111.10
1	P	290	SER	CA-CB-OG	8.25	127.60	111.10
1	Q	245	GLU	CA-CB-CG	8.21	130.52	114.10
1	R	146	ASN	CA-CB-CG	8.17	120.77	112.60
1	R	247	GLU	CA-CB-CG	8.07	130.25	114.10
1	O	199	ALA	N-CA-C	8.05	120.14	111.36
1	O	207	THR	CA-CB-OG1	-8.04	97.55	109.60
1	P	312	ASP	CA-CB-CG	7.95	120.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	98	ARG	CD-NE-CZ	7.93	135.50	124.40
1	P	90	ASP	CA-CB-CG	-7.82	104.78	112.60
1	O	270	ILE	O-C-N	7.80	127.78	121.85
1	R	38	ASN	CA-CB-CG	-7.79	104.81	112.60
1	Q	132	VAL	CA-C-O	-7.76	114.10	120.70
1	Q	184	ILE	CB-CA-C	-7.76	102.11	111.81
1	Q	97	GLY	N-CA-C	-7.75	104.84	114.92
1	R	70	GLU	CA-CB-CG	7.69	129.49	114.10
1	P	171	MET	CA-CB-CG	7.64	129.37	114.10
1	P	159	LYS	CA-C-N	7.61	130.74	120.77
1	P	159	LYS	C-N-CA	7.61	130.74	120.77
1	Q	174	THR	CA-C-O	-7.54	112.02	120.32
1	P	41	ALA	CA-C-N	7.51	130.21	120.44
1	P	41	ALA	C-N-CA	7.51	130.21	120.44
1	Q	84	TRP	CA-C-N	7.51	128.44	120.03
1	Q	84	TRP	C-N-CA	7.51	128.44	120.03
1	R	143	VAL	CA-C-N	7.50	133.63	122.91
1	R	143	VAL	C-N-CA	7.50	133.63	122.91
1	P	312	ASP	N-CA-C	-7.47	97.09	108.67
1	R	191	LYS	O-C-N	7.44	129.82	122.09
1	Q	22	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	O	84	TRP	CA-C-O	7.43	128.29	120.42
1	Q	102	ARG	CD-NE-CZ	-7.41	114.03	124.40
1	Q	32	ASP	CA-C-N	7.40	131.56	120.31
1	Q	32	ASP	C-N-CA	7.40	131.56	120.31
1	Q	162	HIS	CA-CB-CG	-7.35	106.45	113.80
1	Q	245	GLU	CB-CG-CD	7.34	125.07	112.60
1	R	245	GLU	CA-CB-CG	7.33	128.77	114.10
1	R	173	THR	N-CA-CB	7.32	123.10	110.81
1	P	214	VAL	CA-C-N	7.27	130.75	120.28
1	P	214	VAL	C-N-CA	7.27	130.75	120.28
1	Q	104	ASP	CA-C-N	7.26	130.01	120.28
1	Q	104	ASP	C-N-CA	7.26	130.01	120.28
1	O	176	HIS	N-CA-C	7.25	121.26	109.59
1	P	96	THR	N-CA-CB	7.25	121.00	110.20
1	O	192	ASP	CA-CB-CG	7.24	119.84	112.60
1	P	191	LYS	N-CA-CB	7.22	120.74	110.12
1	R	146	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	R	225	LEU	CA-C-O	7.09	129.13	121.11
1	P	6	ASN	CA-C-O	-7.08	113.17	120.54
1	P	62	ASN	O-C-N	7.07	131.68	122.42
1	P	103	GLU	CA-C-O	-7.04	113.09	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	206	THR	O-C-N	-7.03	116.26	123.29
1	P	231	ARG	NE-CZ-NH2	7.03	125.52	119.20
1	Q	102	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	Q	80	GLU	CA-CB-CG	6.99	128.09	114.10
1	R	286	SER	CA-C-O	-6.99	113.51	121.19
1	O	13	ARG	CD-NE-CZ	6.98	134.18	124.40
1	P	210	ALA	CA-C-N	6.98	129.86	120.65
1	P	210	ALA	C-N-CA	6.98	129.86	120.65
1	P	203	ILE	N-CA-CB	6.97	118.95	111.00
1	P	67	ASN	CA-C-O	-6.95	113.52	121.65
1	P	254	GLU	CA-C-N	6.94	129.31	120.56
1	P	254	GLU	C-N-CA	6.94	129.31	120.56
1	Q	262	ALA	CA-C-N	6.93	130.25	120.28
1	Q	262	ALA	C-N-CA	6.93	130.25	120.28
1	P	124	GLU	CB-CG-CD	6.92	124.36	112.60
1	R	99	PHE	CA-CB-CG	-6.89	106.91	113.80
1	Q	22	ASN	CB-CG-ND2	6.89	126.73	116.40
1	R	254	GLU	CA-CB-CG	6.88	127.86	114.10
1	Q	175	VAL	CB-CA-C	6.87	120.74	111.88
1	R	186	ASP	CA-C-O	6.86	128.59	120.70
1	P	100	THR	CA-CB-OG1	-6.84	99.34	109.60
1	R	199	ALA	N-CA-C	6.83	119.31	111.11
1	P	8	PHE	CA-C-O	-6.82	110.76	120.51
1	R	129	VAL	CA-C-N	6.81	130.79	121.05
1	R	129	VAL	C-N-CA	6.81	130.79	121.05
1	O	220	GLU	CA-CB-CG	6.81	127.72	114.10
1	P	77	ARG	CA-C-N	6.81	131.15	122.64
1	P	77	ARG	C-N-CA	6.81	131.15	122.64
1	O	247	GLU	CB-CG-CD	6.80	124.16	112.60
1	Q	298	MET	CA-C-N	6.80	132.65	122.58
1	Q	298	MET	C-N-CA	6.80	132.65	122.58
1	O	208	THR	CA-CB-OG1	-6.80	99.41	109.60
1	O	196	ALA	CA-C-O	6.79	127.81	119.11
1	Q	315	THR	CA-C-N	6.79	127.47	119.94
1	Q	315	THR	C-N-CA	6.79	127.47	119.94
1	O	207	THR	CA-C-O	6.78	129.74	121.94
1	R	157	PHE	CA-CB-CG	6.74	120.54	113.80
1	O	256	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	R	167	ILE	N-CA-CB	6.74	118.68	111.00
1	O	124	GLU	CB-CG-CD	6.72	124.02	112.60
1	P	278	LEU	CA-C-O	-6.71	114.03	121.89
1	R	17	ARG	CD-NE-CZ	6.71	133.79	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	251	THR	CA-C-O	-6.70	113.62	121.46
1	Q	92	VAL	O-C-N	6.69	130.49	123.26
1	O	89	VAL	CB-CA-C	6.66	119.02	110.96
1	O	313	ASN	O-C-N	-6.65	113.75	122.39
1	P	255	VAL	CA-C-O	-6.63	114.14	121.17
1	Q	127	THR	CA-C-O	-6.62	113.17	120.38
1	P	313	ASN	CA-CB-CG	-6.59	106.00	112.60
1	O	4	GLY	CA-C-O	-6.58	115.55	121.47
1	O	104	ASP	CA-CB-CG	-6.58	106.02	112.60
1	P	202	SER	CA-CB-OG	6.58	124.25	111.10
1	R	69	LYS	CB-CA-C	-6.55	99.17	109.84
1	R	174	THR	O-C-N	6.55	131.00	123.27
1	O	241	ASP	CA-CB-CG	6.54	119.14	112.60
1	O	19	ALA	CA-C-N	6.54	129.37	120.54
1	O	19	ALA	C-N-CA	6.54	129.37	120.54
1	Q	25	ILE	N-CA-CB	6.52	123.08	110.95
1	R	135	ASP	CA-CB-CG	-6.52	106.08	112.60
1	R	79	PRO	CA-C-N	6.51	129.30	120.38
1	R	79	PRO	C-N-CA	6.51	129.30	120.38
1	O	157	PHE	CB-CA-C	6.51	120.63	109.24
1	O	175	VAL	CB-CA-C	6.50	120.72	111.81
1	P	184	ILE	CB-CA-C	-6.50	103.66	111.97
1	R	144	ILE	N-CA-C	6.50	118.39	108.71
1	Q	195	ARG	CA-C-N	6.39	131.39	120.72
1	Q	195	ARG	C-N-CA	6.39	131.39	120.72
1	P	323	ASP	CA-CB-CG	6.39	118.99	112.60
1	O	245	GLU	CA-CB-CG	6.38	126.86	114.10
1	Q	254	GLU	CA-CB-CG	6.38	126.86	114.10
1	P	128	ILE	N-CA-C	6.38	117.10	108.17
1	Q	30	VAL	CA-C-O	-6.37	114.53	121.28
1	O	173	THR	N-CA-CB	6.37	121.82	110.80
1	P	168	VAL	CA-C-O	6.37	127.38	120.69
1	Q	230	MET	O-C-N	6.32	131.36	123.14
1	R	226	ASN	N-CA-CB	-6.32	101.73	111.46
1	O	217	VAL	CB-CA-C	6.32	118.81	111.55
1	O	67	ASN	OD1-CG-ND2	6.30	128.90	122.60
1	Q	230	MET	CA-C-O	-6.30	112.31	120.25
1	P	149	CYS	CA-C-N	6.29	129.22	120.29
1	P	149	CYS	C-N-CA	6.29	129.22	120.29
1	P	206	THR	CA-C-O	-6.28	114.70	121.36
1	R	209	GLY	N-CA-C	-6.28	104.88	115.80
1	R	62	ASN	N-CA-CB	6.27	120.08	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	166	GLY	O-C-N	6.26	130.84	122.70
1	Q	37	ALA	CA-C-O	-6.25	113.03	120.10
1	R	307	VAL	CB-CA-C	6.24	118.61	110.12
1	R	67	ASN	CA-CB-CG	6.23	118.83	112.60
1	P	171	MET	N-CA-CB	-6.22	100.35	110.81
1	O	129	VAL	N-CA-CB	6.22	119.74	111.90
1	P	231	ARG	CD-NE-CZ	6.22	133.10	124.40
1	P	252	VAL	O-C-N	6.22	127.90	121.87
1	R	69	LYS	N-CA-CB	6.18	119.53	109.95
1	O	278	LEU	CB-CA-C	6.18	121.14	110.45
1	O	252	VAL	CA-C-N	6.17	128.55	120.28
1	O	252	VAL	C-N-CA	6.17	128.55	120.28
1	R	307	VAL	CA-C-N	6.17	131.22	123.14
1	R	307	VAL	C-N-CA	6.17	131.22	123.14
1	P	158	ALA	CA-C-O	6.16	127.06	119.97
1	O	22	ASN	CA-C-O	6.16	125.59	119.49
1	Q	261	ALA	CA-C-N	6.15	128.44	120.44
1	Q	261	ALA	C-N-CA	6.15	128.44	120.44
1	O	51	GLY	CA-C-N	6.12	129.52	120.95
1	O	51	GLY	C-N-CA	6.12	129.52	120.95
1	R	290	SER	CA-CB-OG	6.12	123.35	111.10
1	R	312	ASP	N-CA-C	-6.10	99.21	108.67
1	O	20	LEU	O-C-N	6.10	128.43	122.09
1	O	5	ILE	CA-C-N	-6.10	114.66	122.77
1	O	5	ILE	C-N-CA	-6.10	114.66	122.77
1	R	204	ILE	CA-CB-CG1	-6.09	100.05	110.40
1	Q	299	VAL	CA-C-N	6.08	131.47	122.71
1	Q	299	VAL	C-N-CA	6.08	131.47	122.71
1	R	246	LEU	N-CA-CB	-6.08	100.73	110.46
1	R	327	TYR	CA-C-N	6.08	128.44	120.60
1	R	327	TYR	C-N-CA	6.08	128.44	120.60
1	R	234	THR	N-CA-C	-6.07	99.68	109.58
1	R	218	LEU	CA-C-N	6.07	125.96	119.28
1	R	218	LEU	C-N-CA	6.07	125.96	119.28
1	P	22	ASN	O-C-N	6.07	129.19	121.12
1	Q	199	ALA	N-CA-C	6.07	118.69	111.71
1	O	304	MET	CA-C-O	-6.06	113.69	120.54
1	P	192	ASP	CA-C-O	-6.05	113.47	120.49
1	R	30	VAL	CA-C-O	-6.05	115.31	121.67
1	O	184	ILE	CB-CA-C	-6.04	104.23	111.97
1	O	85	GLY	CA-C-N	6.03	128.97	120.28
1	O	85	GLY	C-N-CA	6.03	128.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	187	LEU	O-C-N	6.03	126.07	121.85
1	R	26	GLU	CA-C-O	6.03	127.85	120.25
1	O	272	ALA	CA-C-O	-6.03	114.57	121.68
1	Q	176	HIS	N-CA-CB	-6.03	100.99	110.69
1	P	108	HIS	CA-CB-CG	-6.02	107.78	113.80
1	Q	117	ILE	CA-C-N	-6.02	114.84	122.37
1	Q	117	ILE	C-N-CA	-6.02	114.84	122.37
1	O	128	ILE	CA-C-N	6.02	131.19	123.13
1	O	128	ILE	C-N-CA	6.02	131.19	123.13
1	O	4	GLY	N-CA-C	-6.02	101.70	110.90
1	O	164	GLN	N-CA-C	6.01	119.08	111.69
1	O	254	GLU	CA-C-N	6.01	128.13	120.56
1	O	254	GLU	C-N-CA	6.01	128.13	120.56
1	R	53	LEU	CB-CA-C	6.00	119.91	109.65
1	O	315	THR	N-CA-C	5.96	117.57	111.14
1	R	17	ARG	CA-C-N	5.96	128.75	120.29
1	R	17	ARG	C-N-CA	5.96	128.75	120.29
1	P	167	ILE	CA-C-O	-5.96	113.98	120.71
1	R	124	GLU	CB-CG-CD	5.95	122.72	112.60
1	O	111	ALA	N-CA-CB	5.92	119.50	110.44
1	P	171	MET	CB-CA-C	5.92	120.01	109.65
1	R	4	GLY	CA-C-O	5.92	125.56	120.94
1	R	149	CYS	CA-C-N	5.92	128.14	120.44
1	R	149	CYS	C-N-CA	5.92	128.14	120.44
1	R	180	ASN	CA-C-N	5.92	132.41	121.52
1	R	180	ASN	C-N-CA	5.92	132.41	121.52
1	O	197	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	P	102	ARG	CA-C-N	5.92	128.21	120.28
1	P	102	ARG	C-N-CA	5.92	128.21	120.28
1	O	81	ASN	CA-CB-CG	-5.90	106.70	112.60
1	R	137	TYR	O-C-N	5.89	129.93	123.04
1	R	37	ALA	CA-C-O	-5.88	114.32	120.55
1	O	290	SER	O-C-N	5.87	130.43	123.33
1	Q	31	ASN	O-C-N	5.87	130.28	123.30
1	O	132	VAL	CA-C-O	-5.86	115.10	120.73
1	P	199	ALA	N-CA-C	5.86	118.45	111.71
1	O	283	TYR	CA-CB-CG	-5.86	103.35	113.90
1	P	140	ALA	N-CA-CB	-5.86	102.53	110.67
1	R	247	GLU	N-CA-CB	5.86	119.12	110.33
1	P	42	HIS	CA-CB-CG	-5.86	107.94	113.80
1	Q	210	ALA	CA-C-O	-5.85	113.48	120.10
1	R	158	ALA	CA-C-N	5.85	128.37	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	158	ALA	C-N-CA	5.85	128.37	120.65
1	P	30	VAL	CA-C-O	-5.84	114.86	121.75
1	P	230	MET	N-CA-CB	5.84	119.93	110.77
1	Q	266	GLU	N-CA-C	5.83	118.11	111.11
1	P	198	ALA	CA-C-N	5.82	128.66	120.28
1	P	198	ALA	C-N-CA	5.82	128.66	120.28
1	Q	290	SER	CA-CB-OG	5.82	122.74	111.10
1	Q	8	PHE	CA-C-N	-5.82	115.30	122.75
1	Q	8	PHE	C-N-CA	-5.82	115.30	122.75
1	O	121	PRO	N-CA-C	-5.82	101.96	111.21
1	Q	173	THR	CA-CB-CG2	5.82	120.39	110.50
1	P	126	ILE	O-C-N	5.81	128.02	122.97
1	Q	249	GLU	N-CA-CB	5.81	119.74	110.16
1	R	110	GLU	CG-CD-OE1	5.80	131.75	118.40
1	O	38	ASN	CA-CB-CG	-5.80	106.80	112.60
1	Q	160	VAL	CA-C-O	-5.79	115.39	121.41
1	R	281	ARG	N-CA-CB	5.78	119.13	110.22
1	R	146	ASN	CB-CG-ND2	5.78	125.07	116.40
1	P	63	ASN	CB-CG-ND2	5.78	125.06	116.40
1	O	291	THR	N-CA-CB	5.77	119.61	110.84
1	R	254	GLU	O-C-N	5.77	128.02	122.07
1	Q	22	ASN	CA-C-N	5.76	125.30	119.19
1	Q	22	ASN	C-N-CA	5.76	125.30	119.19
1	R	13	ARG	NH1-CZ-NH2	-5.76	111.82	119.30
1	R	62	ASN	CA-C-O	-5.75	112.48	119.32
1	O	56	GLU	N-CA-CB	5.75	119.64	110.16
1	P	226	ASN	CB-CA-C	5.74	122.80	110.45
1	Q	194	ARG	CD-NE-CZ	5.72	132.41	124.40
1	P	158	ALA	N-CA-C	-5.71	105.19	111.82
1	R	204	ILE	CB-CA-C	-5.71	105.65	111.08
1	R	294	ALA	CA-C-O	-5.70	114.47	120.63
1	O	299	VAL	CA-C-N	5.70	131.02	122.75
1	O	299	VAL	C-N-CA	5.70	131.02	122.75
1	P	110	GLU	CG-CD-OE2	-5.70	105.29	118.40
1	P	293	ASP	CA-C-N	5.70	128.19	120.38
1	P	293	ASP	C-N-CA	5.70	128.19	120.38
1	Q	179	THR	CA-CB-OG1	-5.70	101.05	109.60
1	P	31	ASN	CA-CB-CG	-5.69	106.91	112.60
1	P	177	SER	CA-CB-OG	-5.68	99.75	111.10
1	Q	133	ASN	CA-CB-CG	-5.68	106.92	112.60
1	R	112	GLY	N-CA-C	5.67	122.29	114.92
1	O	315	THR	CA-C-N	5.66	126.22	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	315	THR	C-N-CA	5.66	126.22	119.94
1	P	96	THR	CA-C-O	-5.65	113.97	120.24
1	P	198	ALA	CA-C-O	5.65	128.59	120.51
1	O	238	SER	CA-C-O	-5.64	115.19	121.51
1	P	104	ASP	CA-C-O	5.64	126.51	120.70
1	R	177	SER	CA-CB-OG	-5.64	99.82	111.10
1	Q	276	GLU	CA-CB-CG	-5.63	102.84	114.10
1	P	80	GLU	CA-CB-CG	5.62	125.35	114.10
1	Q	291	THR	CA-C-O	-5.62	114.28	120.30
1	R	218	LEU	O-C-N	5.62	126.43	121.32
1	Q	51	GLY	CA-C-N	5.61	128.80	120.95
1	Q	51	GLY	C-N-CA	5.61	128.80	120.95
1	O	226	ASN	N-CA-CB	5.60	120.41	111.56
1	O	252	VAL	O-C-N	5.60	127.30	121.87
1	R	109	LEU	CB-CA-C	5.60	120.37	110.85
1	P	136	LYS	CA-C-N	5.59	128.78	120.95
1	P	136	LYS	C-N-CA	5.59	128.78	120.95
1	P	46	TYR	CA-C-N	5.59	131.78	122.73
1	P	46	TYR	C-N-CA	5.59	131.78	122.73
1	O	176	HIS	CA-CB-CG	-5.58	108.22	113.80
1	P	169	ARG	CD-NE-CZ	5.58	132.22	124.40
1	Q	108	HIS	O-C-N	5.58	128.04	122.12
1	O	183	ARG	CA-C-O	-5.58	114.60	120.80
1	Q	45	LYS	CA-C-O	5.58	126.86	121.00
1	R	190	HIS	CA-C-N	5.58	128.07	120.54
1	R	190	HIS	C-N-CA	5.58	128.07	120.54
1	O	71	ILE	CA-C-O	-5.57	114.13	120.65
1	R	15	VAL	O-C-N	5.56	127.56	121.83
1	P	321	VAL	N-CA-CB	5.56	118.10	110.54
1	P	231	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	P	22	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	Q	47	ASP	CA-C-N	5.56	128.28	120.28
1	Q	47	ASP	C-N-CA	5.56	128.28	120.28
1	P	105	ALA	CA-C-N	5.55	129.99	120.72
1	P	105	ALA	C-N-CA	5.55	129.99	120.72
1	Q	204	ILE	N-CA-CB	-5.55	103.44	111.21
1	O	295	LEU	CA-C-O	-5.54	113.07	119.61
1	R	181	ASP	CB-CG-OD1	5.54	131.15	118.40
1	O	307	VAL	N-CA-C	-5.54	100.20	108.46
1	R	55	ALA	O-C-N	5.54	129.43	123.56
1	R	207	THR	CA-CB-OG1	-5.54	101.30	109.60
1	R	58	SER	CA-C-N	5.53	130.05	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	58	SER	C-N-CA	5.53	130.05	123.19
1	Q	249	GLU	N-CA-C	-5.53	100.28	109.46
1	O	245	GLU	CB-CG-CD	5.52	121.99	112.60
1	Q	177	SER	CA-C-O	-5.51	115.70	121.55
1	R	81	ASN	CA-C-O	-5.51	112.61	119.28
1	Q	52	ARG	CD-NE-CZ	-5.51	116.69	124.40
1	R	191	LYS	N-CA-C	-5.49	104.52	111.11
1	O	301	ASP	CA-CB-CG	-5.49	107.11	112.60
1	P	319	HIS	CB-CA-C	5.49	120.18	110.85
1	R	222	LYS	CA-C-N	5.49	131.67	120.80
1	R	222	LYS	C-N-CA	5.49	131.67	120.80
1	R	162	HIS	N-CA-CB	5.47	117.95	110.01
1	O	312	ASP	CA-C-O	-5.46	115.08	120.98
1	P	245	GLU	CB-CG-CD	5.46	121.89	112.60
1	P	285	GLY	CA-C-N	5.46	129.10	121.02
1	P	285	GLY	C-N-CA	5.46	129.10	121.02
1	Q	138	ASP	CA-CB-CG	5.46	118.06	112.60
1	O	2	LYS	CA-C-N	5.46	130.86	122.68
1	O	2	LYS	C-N-CA	5.46	130.86	122.68
1	P	241	ASP	CA-CB-CG	5.45	118.05	112.60
1	Q	127	THR	O-C-N	5.44	129.71	123.29
1	Q	159	LYS	CA-C-N	5.44	127.89	120.77
1	Q	159	LYS	C-N-CA	5.44	127.89	120.77
1	P	150	THR	N-CA-CB	5.43	118.20	110.16
1	R	169	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	R	288	VAL	CA-CB-CG1	5.43	119.63	110.40
1	O	305	VAL	CA-C-N	5.42	130.64	122.99
1	O	305	VAL	C-N-CA	5.42	130.64	122.99
1	P	319	HIS	CA-C-N	5.41	127.48	120.44
1	P	319	HIS	C-N-CA	5.41	127.48	120.44
1	R	158	ALA	N-CA-C	-5.41	105.41	112.23
1	R	68	GLY	CA-C-O	-5.41	113.58	119.59
1	R	175	VAL	N-CA-C	-5.41	98.87	107.15
1	R	133	ASN	CA-C-O	-5.41	114.81	120.32
1	R	269	GLY	CA-C-N	5.39	131.68	121.97
1	R	269	GLY	C-N-CA	5.39	131.68	121.97
1	Q	103	GLU	CA-CB-CG	5.39	124.88	114.10
1	Q	6	ASN	O-C-N	5.38	129.45	123.05
1	P	328	ILE	CA-CB-CG2	5.38	119.64	110.50
1	P	34	THR	CA-CB-OG1	-5.37	101.55	109.60
1	R	175	VAL	O-C-N	5.37	128.90	122.62
1	Q	313	ASN	CA-C-O	-5.36	113.00	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	0	ALA	CA-C-O	-5.36	111.69	120.80
1	O	162	HIS	CA-CB-CG	-5.36	108.44	113.80
1	P	103	GLU	O-C-N	5.36	127.80	122.12
1	Q	135	ASP	CA-CB-CG	5.35	117.95	112.60
1	O	127	THR	N-CA-CB	5.34	119.12	110.42
1	P	47	ASP	CA-CB-CG	-5.34	107.26	112.60
1	R	40	LEU	CB-CA-C	5.34	119.66	110.79
1	R	108	HIS	N-CA-CB	5.34	118.56	110.28
1	P	178	TYR	CA-C-O	5.34	127.21	121.55
1	P	86	GLU	CA-C-O	-5.33	112.82	119.38
1	P	173	THR	N-CA-CB	5.33	120.65	111.00
1	P	26	GLU	CA-C-O	-5.33	113.54	120.25
1	Q	72	ILE	CA-C-O	-5.32	114.97	121.04
1	P	123	ASN	CB-CG-ND2	-5.32	108.43	116.40
1	O	181	ASP	N-CA-CB	-5.31	101.48	110.41
1	P	118	ILE	O-C-N	5.31	129.42	122.94
1	O	249	GLU	N-CA-C	-5.31	101.81	110.20
1	R	11	ILE	CA-C-O	-5.31	115.43	120.95
1	Q	276	GLU	OE1-CD-OE2	5.30	135.63	122.90
1	O	176	HIS	N-CA-CB	-5.30	102.15	110.69
1	R	132	VAL	CA-C-O	-5.30	114.37	120.83
1	R	194	ARG	CA-C-N	5.30	131.66	121.18
1	R	194	ARG	C-N-CA	5.30	131.66	121.18
1	R	169	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	R	230	MET	N-CA-CB	5.29	119.50	110.87
1	R	301	ASP	N-CA-CB	-5.29	103.96	111.84
1	P	322	VAL	CA-C-O	-5.28	115.46	120.95
1	P	70	GLU	CB-CG-CD	5.28	121.58	112.60
1	Q	155	ALA	CB-CA-C	5.28	120.58	110.17
1	P	59	VAL	CB-CA-C	5.28	118.84	110.81
1	R	250	VAL	CA-C-O	5.28	127.27	121.67
1	Q	78	ASP	CA-C-N	5.27	125.58	119.47
1	Q	78	ASP	C-N-CA	5.27	125.58	119.47
1	P	157	PHE	CA-CB-CG	5.26	119.06	113.80
1	P	318	SER	CA-CB-OG	-5.26	100.58	111.10
1	R	159	LYS	CA-C-N	5.26	127.28	120.70
1	R	159	LYS	C-N-CA	5.26	127.28	120.70
1	O	140	ALA	O-C-N	5.25	129.37	122.33
1	Q	154	LEU	N-CA-CB	-5.25	102.36	110.13
1	P	62	ASN	CA-C-O	-5.24	113.17	119.15
1	Q	320	ARG	CD-NE-CZ	5.24	131.73	124.40
1	Q	17	ARG	NE-CZ-NH1	-5.23	116.27	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	8	PHE	CA-C-N	5.23	129.17	121.96
1	R	8	PHE	C-N-CA	5.23	129.17	121.96
1	R	103	GLU	N-CA-CB	5.23	118.27	110.22
1	O	31	ASN	CB-CA-C	5.22	118.83	110.16
1	P	123	ASN	CA-CB-CG	-5.22	107.38	112.60
1	Q	102	ARG	CB-CG-CD	5.22	123.32	111.30
1	R	287	THR	CA-CB-OG1	-5.22	101.77	109.60
1	R	179	THR	CA-CB-OG1	-5.22	101.77	109.60
1	P	5	ILE	CA-C-N	-5.22	116.06	122.84
1	P	5	ILE	C-N-CA	-5.22	116.06	122.84
1	Q	30	VAL	O-C-N	5.22	128.95	123.00
1	R	27	VAL	CB-CA-C	5.21	117.03	111.35
1	P	160	VAL	CA-C-O	-5.21	115.99	121.41
1	Q	44	LEU	CA-C-N	5.21	127.53	120.65
1	Q	44	LEU	C-N-CA	5.21	127.53	120.65
1	R	139	LYS	N-CA-CB	5.21	117.78	110.12
1	P	239	VAL	CA-CB-CG1	5.21	119.25	110.40
1	P	95	SER	CA-CB-OG	-5.21	100.69	111.10
1	P	173	THR	CA-C-N	-5.21	115.82	123.00
1	P	173	THR	C-N-CA	-5.21	115.82	123.00
1	Q	122(A)	LYS	N-CA-CB	5.20	118.93	110.77
1	O	123	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	O	325	ALA	CA-C-N	5.20	128.21	120.31
1	O	325	ALA	C-N-CA	5.20	128.21	120.31
1	P	40	LEU	O-C-N	-5.20	115.88	122.27
1	R	293	ASP	CA-C-N	5.20	127.50	120.38
1	R	293	ASP	C-N-CA	5.20	127.50	120.38
1	Q	174	THR	O-C-N	5.19	129.39	123.27
1	Q	297	THR	CA-C-N	5.19	130.85	122.29
1	Q	297	THR	C-N-CA	5.19	130.85	122.29
1	P	97	GLY	CA-C-N	5.18	130.88	121.92
1	P	97	GLY	C-N-CA	5.18	130.88	121.92
1	Q	55	ALA	CA-C-O	-5.17	113.11	120.51
1	O	183	ARG	NE-CZ-NH2	-5.17	114.54	119.20
1	R	166	GLY	CA-C-N	5.17	128.84	122.37
1	R	166	GLY	C-N-CA	5.17	128.84	122.37
1	O	251	THR	N-CA-CB	5.17	120.54	111.55
1	O	212	LYS	CA-C-N	5.16	128.86	120.60
1	O	212	LYS	C-N-CA	5.16	128.86	120.60
1	O	94	GLU	CB-CA-C	5.16	120.07	111.30
1	O	183	ARG	O-C-N	5.16	129.23	123.19
1	Q	25	ILE	CA-CB-CG2	5.16	119.26	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	70	GLU	N-CA-CB	5.15	117.93	109.95
1	P	22	ASN	CA-C-O	-5.14	114.78	119.62
1	O	198	ALA	CA-C-O	-5.14	116.05	120.88
1	P	228	MET	CA-CB-CG	-5.14	103.81	114.10
1	R	168	VAL	CB-CA-C	5.14	118.73	111.94
1	R	314	GLU	CB-CA-C	5.14	118.83	110.24
1	P	321	VAL	O-C-N	5.14	126.85	121.87
1	P	322	VAL	O-C-N	5.13	126.85	121.87
1	P	137	TYR	CA-C-N	-5.13	116.23	122.64
1	P	137	TYR	C-N-CA	-5.13	116.23	122.64
1	P	98	ARG	CD-NE-CZ	5.13	131.58	124.40
1	P	237	VAL	CA-CB-CG1	5.13	119.11	110.40
1	R	319	HIS	CA-CB-CG	-5.13	108.67	113.80
1	O	108	HIS	N-CA-CB	5.12	118.90	110.39
1	Q	221	LEU	CA-C-N	5.12	129.40	121.26
1	Q	221	LEU	C-N-CA	5.12	129.40	121.26
1	R	192	ASP	CA-CB-CG	5.11	117.71	112.60
1	R	131	GLY	N-CA-C	-5.10	107.61	114.25
1	P	184	ILE	O-C-N	5.10	126.91	121.91
1	Q	113	ALA	N-CA-C	-5.10	102.22	110.32
1	O	194	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	O	312	ASP	N-CA-C	-5.09	99.47	108.23
1	P	245	GLU	CA-C-O	-5.09	114.73	120.43
1	P	133	ASN	CA-C-O	-5.08	116.44	121.02
1	O	254	GLU	CB-CG-CD	5.08	121.24	112.60
1	O	204	ILE	O-C-N	5.07	126.88	121.10
1	P	164	GLN	N-CA-C	5.07	116.61	111.14
1	P	44	LEU	CA-C-N	5.07	127.33	120.44
1	P	44	LEU	C-N-CA	5.07	127.33	120.44
1	P	275	GLU	CB-CG-CD	5.07	121.21	112.60
1	Q	17	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	R	280	SER	CA-C-O	-5.07	115.16	120.63
1	Q	9	GLY	N-CA-C	-5.06	103.96	112.77
1	O	186	ASP	CA-C-O	5.06	127.75	120.51
1	Q	176	HIS	CA-C-N	5.06	128.39	120.75
1	Q	176	HIS	C-N-CA	5.06	128.39	120.75
1	P	236	ASN	CB-CA-C	5.05	118.13	109.99
1	P	305	VAL	CA-C-N	5.05	130.12	123.00
1	P	305	VAL	C-N-CA	5.05	130.12	123.00
1	O	328	ILE	O-C-N	5.05	126.99	121.94
1	Q	26	GLU	O-C-N	5.05	129.10	123.40
1	P	135	ASP	CA-C-O	-5.04	114.17	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	279	VAL	CA-C-O	-5.04	116.53	121.67
1	Q	109	LEU	N-CA-C	-5.04	105.78	111.28
1	P	11	ILE	O-C-N	5.03	126.84	121.91
1	Q	100	THR	N-CA-CB	5.03	118.35	110.46
1	P	190	HIS	CA-C-O	-5.02	115.37	120.89
1	O	249	GLU	CA-C-N	-5.01	116.59	123.46
1	O	249	GLU	C-N-CA	-5.01	116.59	123.46
1	Q	56	GLU	CB-CG-CD	5.01	121.12	112.60
1	R	260	LYS	CA-C-N	5.01	127.26	120.44
1	R	260	LYS	C-N-CA	5.01	127.26	120.44
1	P	313	ASN	OD1-CG-ND2	5.01	127.61	122.60
1	Q	249	GLU	CA-CB-CG	5.01	124.12	114.10
1	O	196	ALA	CA-C-N	5.01	129.50	122.09
1	O	196	ALA	C-N-CA	5.01	129.50	122.09
1	P	180	ASN	CA-C-N	5.00	129.90	121.14
1	P	180	ASN	C-N-CA	5.00	129.90	121.14
1	Q	259	LEU	CA-C-O	-5.00	115.57	120.82
1	R	226	ASN	OD1-CG-ND2	5.00	127.60	122.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2525	0	2572	68	0
1	P	2525	0	2572	66	0
1	Q	2525	0	2572	66	0
1	R	2525	0	2572	60	0
2	O	10	0	0	0	0
2	P	10	0	0	0	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	O	114	0	0	5	0
3	P	127	0	0	3	0
3	Q	121	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	142	0	0	6	0
All	All	10644	0	10288	234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (234) 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:O:304:MET:HG2	1:P:171:MET:HE2	1.49	0.94
1:R:176:HIS:HA	1:R:238:SER:HB3	1.56	0.88
1:P:103:GLU:HG3	3:P:438:HOH:O	1.79	0.80
1:Q:144:ILE:HD13	1:Q:328:ILE:HD11	1.63	0.77
1:P:172:MET:HE2	1:P:208:THR:HG21	1.68	0.75
1:O:144:ILE:HD13	1:O:328:ILE:HD11	1.69	0.75
1:Q:221:LEU:HA	1:Q:224:LYS:HD2	1.66	0.75
1:P:187:LEU:HD23	3:Q:363:HOH:O	1.87	0.73
1:O:304:MET:HG2	1:P:171:MET:CE	2.19	0.73
1:Q:306:LYS:HE2	1:R:171:MET:HG3	1.70	0.72
1:Q:184:ILE:HG22	1:Q:185:LEU:HG	1.71	0.71
1:O:271:LEU:HD12	1:O:290:SER:HB3	1.73	0.71
1:O:186:ASP:HA	1:O:196:ALA:O	1.90	0.71
1:O:181:ASP:OD1	1:O:195:ARG:NH1	2.23	0.70
1:O:306:LYS:HE2	1:P:171:MET:HG3	1.75	0.69
1:R:103:GLU:HG3	3:R:459:HOH:O	1.92	0.69
1:O:11:ILE:O	1:O:15:VAL:HG23	1.92	0.69
1:Q:2:LYS:HD3	1:Q:28:VAL:HG11	1.76	0.67
1:Q:19:ALA:CB	1:Q:25:ILE:HD11	2.24	0.67
1:P:130:MET:HE1	1:P:327:TYR:HB2	1.77	0.66
1:O:171:MET:HG3	1:P:306:LYS:HE2	1.76	0.66
1:Q:181:ASP:OD1	1:Q:195:ARG:HD3	1.95	0.65
1:P:181:ASP:OD1	1:P:195:ARG:NH1	2.29	0.65
1:R:172:MET:HE3	1:R:208:THR:HG21	1.79	0.65
1:Q:78:ASP:OD1	1:Q:80:GLU:HB2	1.97	0.64
1:R:172:MET:HE1	1:R:210:ALA:HB3	1.80	0.64
1:R:246:LEU:HB2	1:R:303:LYS:O	1.96	0.64
1:P:129:VAL:HG23	1:P:217:VAL:HG11	1.78	0.64
1:Q:182:GLN:HB3	3:Q:368:HOH:O	1.97	0.63
3:O:353:HOH:O	1:R:187:LEU:HD23	1.96	0.63
1:P:150:THR:HG21	1:P:172:MET:HE1	1.80	0.63
1:Q:171:MET:HE2	1:R:304:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:165:PHE:HA	1:R:248:LYS:HD2	1.80	0.62
1:Q:19:ALA:HB2	1:Q:25:ILE:HD11	1.82	0.62
1:O:260:LYS:HD2	1:O:273:TYR:CE2	2.35	0.61
1:O:172:MET:CE	1:O:208:THR:HG21	2.29	0.61
1:O:251:THR:OG1	1:O:254:GLU:HG3	2.02	0.60
1:Q:144:ILE:CD1	1:Q:328:ILE:HD11	2.31	0.60
1:P:237:VAL:HG11	1:P:283:TYR:HB2	1.84	0.59
1:Q:211:ALA:HB3	3:Q:352:HOH:O	2.02	0.59
1:R:186:ASP:HA	1:R:196:ALA:O	2.02	0.59
1:P:17:ARG:HG2	1:P:53:LEU:HD13	1.84	0.59
1:O:26:GLU:OE1	1:O:28:VAL:HG12	2.03	0.59
1:P:186:ASP:OD1	1:P:197:ARG:HA	2.03	0.59
1:R:283:TYR:O	1:R:286:SER:HB2	2.02	0.59
1:R:240:VAL:O	1:R:308:VAL:HA	2.03	0.58
1:O:169:ARG:HD3	1:P:301:ASP:HB2	1.86	0.58
1:Q:310:TRP:HZ2	1:R:205:PRO:HG2	1.68	0.58
1:Q:171:MET:CG	1:R:306:LYS:HE2	2.34	0.58
1:P:186:ASP:HB2	1:Q:10:ARG:NH1	2.19	0.57
1:R:176:HIS:HA	1:R:238:SER:CB	2.33	0.57
1:O:56:GLU:H	1:O:67:ASN:ND2	2.02	0.57
1:P:79:PRO:HA	1:P:82:LEU:HD12	1.86	0.57
1:O:57:VAL:HA	1:O:65:VAL:O	2.06	0.56
1:O:115:LYS:HE3	1:O:137:TYR:OH	2.06	0.56
1:P:186:ASP:HB2	1:Q:10:ARG:HH12	1.71	0.56
1:R:170:GLY:O	1:R:225:LEU:HA	2.06	0.56
1:Q:171:MET:HG2	1:R:306:LYS:HE2	1.88	0.56
1:Q:273:TYR:HB3	3:Q:422:HOH:O	2.05	0.56
1:Q:283:TYR:O	1:Q:286:SER:HB3	2.06	0.56
1:R:182:GLN:HB3	3:R:372:HOH:O	2.06	0.56
1:Q:90:ASP:OD1	1:Q:114:LYS:HE3	2.04	0.56
1:P:130:MET:HE1	1:P:327:TYR:CB	2.36	0.55
1:O:188:PRO:HD3	3:R:367:HOH:O	2.06	0.55
1:P:179:THR:OG1	1:P:181:ASP:HB3	2.06	0.55
1:R:2:LYS:HE2	1:R:28:VAL:HG11	1.89	0.55
1:P:6:ASN:OD1	1:P:31:ASN:HB3	2.07	0.55
1:P:101:LYS:HB2	3:P:420:HOH:O	2.07	0.54
1:Q:56:GLU:H	1:Q:67:ASN:ND2	2.05	0.54
1:Q:176:HIS:O	1:Q:231:ARG:HA	2.07	0.54
1:R:260:LYS:O	1:R:264:GLU:HG3	2.08	0.54
1:Q:82:LEU:O	1:Q:83:ALA:C	2.48	0.54
1:O:237:VAL:HG11	1:O:283:TYR:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:168:VAL:CG2	1:O:247:GLU:HG2	2.39	0.53
1:O:184:ILE:HD11	1:R:182:GLN:O	2.08	0.53
1:R:176:HIS:ND1	1:R:177:SER:O	2.36	0.53
1:Q:301:ASP:HB2	1:R:169:ARG:HD3	1.90	0.53
1:O:211:ALA:HB3	3:O:343:HOH:O	2.08	0.53
1:Q:319:HIS:HE1	3:Q:434:HOH:O	1.90	0.53
1:R:0:ALA:HB3	1:R:24:ASP:O	2.09	0.53
1:P:200:ALA:HA	1:P:233:PRO:HB3	1.91	0.53
1:R:19:ALA:HB2	1:R:25:ILE:HD11	1.90	0.52
1:R:287:THR:HG22	1:R:319:HIS:CE1	2.44	0.52
1:O:298:MET:O	1:O:305:VAL:HG23	2.08	0.52
1:O:176:HIS:HB3	1:O:231:ARG:HD3	1.92	0.52
1:Q:172:MET:CE	1:Q:208:THR:HG21	2.39	0.52
1:R:288:VAL:HG23	1:R:290:SER:H	1.75	0.52
1:P:315:THR:O	1:P:316:GLY:C	2.53	0.51
1:O:168:VAL:HG12	1:O:169:ARG:HG2	1.91	0.51
1:Q:17:ARG:HG2	1:Q:53:LEU:HD13	1.91	0.51
1:Q:19:ALA:HB1	1:Q:25:ILE:HD11	1.90	0.51
1:O:36:ASP:OD1	1:O:38:ASN:HB2	2.11	0.51
1:O:301:ASP:HB2	1:P:169:ARG:HD3	1.92	0.51
1:O:2:LYS:HD3	1:O:28:VAL:HG11	1.93	0.51
1:R:45:LYS:O	1:R:52:ARG:HA	2.11	0.51
1:Q:310:TRP:CZ2	1:R:205:PRO:HG2	2.46	0.51
1:P:34:THR:HG22	1:P:39:THR:HB	1.93	0.51
1:P:98:ARG:HG3	1:P:98:ARG:HH11	1.76	0.50
1:O:78:ASP:OD1	1:O:80:GLU:HG3	2.11	0.50
1:P:178:TYR:HA	1:P:182:GLN:OE1	2.12	0.50
1:Q:132:VAL:HG13	1:Q:218:LEU:HD21	1.93	0.50
1:R:79:PRO:HA	1:R:82:LEU:HD12	1.93	0.49
1:P:78:ASP:OD2	1:P:80:GLU:HB2	2.12	0.49
1:Q:41:ALA:HB2	1:Q:64:LEU:CD2	2.43	0.49
1:Q:299:VAL:HA	1:Q:304:MET:O	2.12	0.49
1:Q:178:TYR:HA	1:Q:182:GLN:OE1	2.12	0.49
1:O:20:LEU:HD11	1:O:53:LEU:HD11	1.94	0.49
1:O:45:LYS:HB3	1:O:46:TYR:CD2	2.48	0.49
1:O:300:ILE:HD11	1:P:226:ASN:HB2	1.95	0.49
1:R:104:ASP:O	1:R:107:LYS:HG3	2.13	0.49
1:R:181:ASP:OD1	1:R:195:ARG:HD3	2.13	0.49
1:O:182:GLN:HB3	3:O:357:HOH:O	2.11	0.48
1:R:181:ASP:OD1	1:R:195:ARG:NH1	2.44	0.48
1:Q:144:ILE:HD13	1:Q:328:ILE:CD1	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:146:ASN:ND2	3:R:376:HOH:O	2.45	0.48
1:Q:219:PRO:O	1:Q:222:LYS:HB2	2.12	0.48
1:R:20:LEU:CD1	1:R:53:LEU:HD11	2.44	0.48
1:O:243:VAL:HA	1:O:305:VAL:O	2.14	0.48
1:P:186:ASP:HA	1:P:196:ALA:O	2.13	0.48
1:R:99:PHE:HD1	1:R:104:ASP:HB3	1.78	0.48
1:Q:271:LEU:HD12	1:Q:290:SER:HB3	1.94	0.48
1:R:20:LEU:HD12	1:R:53:LEU:HD11	1.96	0.48
1:Q:306:LYS:HB2	1:R:171:MET:HE3	1.95	0.48
1:P:187:LEU:O	1:P:196:ALA:HB1	2.13	0.48
1:Q:99:PHE:CD1	1:Q:104:ASP:HB3	2.50	0.47
1:P:79:PRO:HA	1:P:82:LEU:CD1	2.45	0.47
1:Q:14:ASN:HB3	1:Q:318:SER:OG	2.15	0.47
1:Q:31:ASN:CG	1:Q:82:LEU:HD21	2.40	0.47
1:O:82:LEU:O	1:O:83:ALA:C	2.57	0.46
1:O:281:ARG:HG2	1:P:202:SER:OG	2.15	0.46
1:R:119:SER:O	1:R:120:ALA:HB2	2.15	0.46
1:O:276:GLU:HB2	1:O:278:LEU:HG	1.96	0.46
1:P:129:VAL:CG2	1:P:217:VAL:HG11	2.43	0.46
1:P:151:THR:OG1	1:P:210:ALA:HA	2.14	0.46
1:O:301:ASP:HB2	1:P:169:ARG:CD	2.46	0.46
1:P:155:ALA:HB3	1:P:156:PRO:HD3	1.98	0.46
1:O:3:VAL:HA	1:O:91:ILE:O	2.15	0.46
1:R:34:THR:HG22	1:R:39:THR:HB	1.97	0.46
1:O:300:ILE:HD11	1:P:226:ASN:CB	2.45	0.46
1:O:144:ILE:HD13	1:O:328:ILE:CD1	2.43	0.46
1:O:186:ASP:OD1	1:O:197:ARG:HA	2.16	0.46
1:P:276:GLU:HB3	1:P:277:PRO:HD2	1.98	0.45
1:R:78:ASP:HB2	3:R:469:HOH:O	2.16	0.45
1:O:20:LEU:CD1	1:O:53:LEU:HD11	2.47	0.45
1:Q:41:ALA:HB2	1:Q:64:LEU:HD22	1.98	0.45
1:O:168:VAL:HG22	1:O:247:GLU:HG2	1.98	0.45
1:Q:99:PHE:HD1	1:Q:104:ASP:HB3	1.81	0.45
1:Q:45:LYS:O	1:Q:52:ARG:HA	2.17	0.45
1:O:127:THR:OG1	1:O:145:SER:HB3	2.16	0.45
1:P:28:VAL:HG22	1:P:89:VAL:CG2	2.46	0.45
1:Q:103:GLU:CD	1:Q:103:GLU:H	2.25	0.45
1:R:129:VAL:HG11	1:R:155:ALA:HB3	1.99	0.45
1:R:204:ILE:HA	1:R:205:PRO:HD3	1.82	0.45
1:O:74:LYS:HE3	1:O:82:LEU:O	2.18	0.44
1:O:273:TYR:CE1	1:O:294:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:328:ILE:HD13	1:Q:328:ILE:HG21	1.80	0.44
1:R:236:ASN:ND2	1:R:312:ASP:OD2	2.43	0.44
1:O:53:LEU:HG	1:O:55:ALA:HB3	1.98	0.44
1:P:184:ILE:HG22	1:P:185:LEU:HG	1.98	0.44
1:P:129:VAL:HG11	1:P:155:ALA:HB3	1.99	0.44
1:P:165:PHE:CD2	1:P:250:VAL:HG11	2.53	0.44
1:P:328:ILE:O	1:P:329:ALA:C	2.60	0.44
1:O:103:GLU:CD	1:O:103:GLU:H	2.25	0.44
1:R:138(A):PRO:HG3	1:R:331:LYS:HB3	2.00	0.44
1:O:44:LEU:HG	1:O:53:LEU:HD22	1.98	0.44
1:P:79:PRO:HB3	1:P:108:HIS:CE1	2.52	0.43
1:Q:168:VAL:HB	1:Q:245:GLU:HB3	1.99	0.43
1:R:253:GLU:CD	1:R:253:GLU:H	2.26	0.43
1:O:79:PRO:HA	1:O:82:LEU:CD1	2.49	0.43
1:O:204:ILE:HG12	1:P:279:VAL:HG11	2.00	0.43
1:O:1:VAL:HG12	1:O:24:ASP:O	2.19	0.43
1:P:293:ASP:OD1	1:P:296:SER:OG	2.31	0.43
1:P:171:MET:HA	1:P:226:ASN:O	2.19	0.43
1:P:231:ARG:HG3	1:P:231:ARG:HH21	1.83	0.43
1:O:180:ASN:HB2	1:R:187:LEU:HD11	2.00	0.43
1:Q:267:LEU:O	1:Q:268:LYS:C	2.60	0.43
1:R:305:VAL:HG22	1:R:307:VAL:HG23	2.01	0.43
1:O:79:PRO:HG2	1:O:107:LYS:HD2	2.00	0.43
1:O:197:ARG:O	1:O:198:ALA:C	2.62	0.42
1:P:128:ILE:HD11	1:P:137:TYR:HB2	2.00	0.42
1:P:201:GLU:CD	1:Q:235:PRO:HG3	2.44	0.42
1:R:263:ALA:O	1:R:268:LYS:HA	2.19	0.42
1:P:329:ALA:HA	1:P:333:LEU:HD22	2.02	0.42
1:Q:172:MET:HE3	1:Q:208:THR:HG21	2.01	0.42
1:R:19:ALA:CB	1:R:25:ILE:HD11	2.49	0.42
1:R:20:LEU:HA	1:R:20:LEU:HD23	1.76	0.42
1:O:275:GLU:HB2	3:O:391:HOH:O	2.18	0.42
1:P:20:LEU:HD12	1:P:53:LEU:HD11	2.02	0.42
1:O:281:ARG:NH1	3:O:434:HOH:O	2.32	0.42
1:P:104:ASP:O	1:P:107:LYS:HG3	2.20	0.42
1:Q:138:ASP:HA	1:Q:138(A):PRO:HD2	1.83	0.42
1:P:220:GLU:HG3	3:P:450:HOH:O	2.19	0.42
1:Q:76:GLU:HB2	1:Q:82:LEU:HD21	2.01	0.42
1:Q:41:ALA:O	1:Q:45:LYS:HB2	2.20	0.42
1:Q:144:ILE:CD1	1:Q:328:ILE:CD1	2.97	0.42
1:Q:242:LEU:O	1:Q:306:LYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:184:ILE:HD13	1:O:184:ILE:HG21	1.81	0.42
1:O:304:MET:HE3	1:O:304:MET:HB2	1.96	0.42
1:P:138:ASP:HA	1:P:138(A):PRO:HD2	1.92	0.42
1:O:29:ALA:HA	1:O:72:ILE:O	2.20	0.41
1:O:83:ALA:HB1	1:O:86:GLU:HG3	2.02	0.41
1:P:333:LEU:HD12	1:P:333:LEU:HA	1.93	0.41
1:Q:171:MET:HG3	1:R:306:LYS:HE2	2.02	0.41
1:Q:331:LYS:HB2	3:Q:441:HOH:O	2.19	0.41
1:R:64:LEU:O	1:R:70:GLU:HA	2.20	0.41
1:R:220:GLU:HG3	3:R:470:HOH:O	2.19	0.41
1:P:176:HIS:HB3	1:P:231:ARG:HD3	2.01	0.41
1:P:289:SER:HG	1:P:320:ARG:HD2	1.86	0.41
1:R:244:ALA:O	1:R:305:VAL:HG12	2.20	0.41
1:R:103:GLU:H	1:R:103:GLU:CD	2.28	0.41
1:Q:54:ASP:O	1:Q:55:ALA:HB2	2.21	0.41
1:Q:301:ASP:HB2	1:R:169:ARG:CD	2.50	0.41
1:O:99:PHE:O	1:O:105:ALA:HB2	2.20	0.41
1:P:67:ASN:HD22	1:P:67:ASN:HA	1.68	0.41
1:P:190:HIS:ND1	1:P:191:LYS:N	2.69	0.41
1:Q:1:VAL:HG21	1:Q:329:ALA:HB2	2.02	0.41
1:Q:20:LEU:HD12	1:Q:53:LEU:HD11	2.03	0.41
1:Q:165:PHE:CD2	1:Q:250:VAL:HG11	2.56	0.41
1:Q:205:PRO:HB3	1:Q:228:MET:CE	2.51	0.41
1:R:130:MET:HE1	1:R:327:TYR:CB	2.51	0.41
1:R:286:SER:O	1:R:315:THR:HB	2.21	0.41
1:O:56:GLU:H	1:O:67:ASN:HD21	1.67	0.40
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.56	0.40
1:O:84:TRP:CE3	1:O:89:VAL:HG11	2.55	0.40
1:Q:300:ILE:HG21	1:Q:300:ILE:HD13	1.75	0.40
1:P:172:MET:CE	1:P:208:THR:HG21	2.45	0.40
1:P:300:ILE:HD13	1:P:300:ILE:HG21	1.86	0.40
1:Q:314:GLU:HG2	3:Q:438:HOH:O	2.21	0.40
1:O:298:MET:HB2	1:O:298:MET:HE3	1.74	0.40
1:P:1:VAL:HG21	1:P:329:ALA:HB2	2.03	0.40
1:O:126:ILE:HG12	1:O:128:ILE:HG13	2.04	0.40
1:P:247:GLU:O	1:P:303:LYS:HE2	2.22	0.40
1:Q:17:ARG:HH11	1:Q:17:ARG:HD3	1.50	0.40
1:R:184:ILE:HG22	1:R:185:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	332/334 (99%)	309 (93%)	20 (6%)	3 (1%)	14	27
1	P	332/334 (99%)	314 (95%)	15 (4%)	3 (1%)	14	27
1	Q	332/334 (99%)	319 (96%)	10 (3%)	3 (1%)	14	27
1	R	332/334 (99%)	311 (94%)	17 (5%)	4 (1%)	10	20
All	All	1328/1336 (99%)	1253 (94%)	62 (5%)	13 (1%)	12	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	237	VAL
1	P	237	VAL
1	Q	166	GLY
1	Q	237	VAL
1	R	237	VAL
1	R	302	GLY
1	Q	198	ALA
1	R	120	ALA
1	P	120	ALA
1	P	198	ALA
1	O	302	GLY
1	O	166	GLY
1	R	166	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	R	339	-	4,4,4	0.65	0	6,6,6	0.34	0
2	SO4	O	338	-	4,4,4	0.83	0	6,6,6	0.29	0
2	SO4	P	338	-	4,4,4	0.79	0	6,6,6	0.31	0
2	SO4	O	339	-	4,4,4	0.74	0	6,6,6	0.33	0
2	SO4	R	338	-	4,4,4	0.71	0	6,6,6	0.34	0
2	SO4	Q	338	-	4,4,4	0.70	0	6,6,6	0.39	0
2	SO4	Q	339	-	4,4,4	0.70	0	6,6,6	0.38	0
2	SO4	P	339	-	4,4,4	0.81	0	6,6,6	0.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	334/334 (100%)	-0.40	0 100 100	5, 16, 38, 55	0
1	P	334/334 (100%)	-0.38	0 100 100	4, 15, 38, 59	0
1	Q	334/334 (100%)	-0.37	3 (0%) 81 78	3, 16, 40, 55	0
1	R	334/334 (100%)	-0.40	0 100 100	3, 15, 36, 51	0
All	All	1336/1336 (100%)	-0.39	3 (0%) 91 89	3, 16, 38, 59	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	332	GLY	2.6
1	Q	180	ASN	2.3
1	Q	103	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	P	339	5/5	0.85	0.29	35,36,37,37	5
2	SO4	O	339	5/5	0.86	0.21	32,33,33,33	5
2	SO4	O	338	5/5	0.89	0.18	32,32,33,34	5
2	SO4	Q	338	5/5	0.90	0.18	35,36,36,36	5
2	SO4	Q	339	5/5	0.90	0.26	33,33,33,35	5
2	SO4	R	338	5/5	0.92	0.22	37,37,37,38	5
2	SO4	R	339	5/5	0.92	0.24	30,30,32,32	5
2	SO4	P	338	5/5	0.94	0.15	32,33,34,35	5

6.5 Other polymers [i](#)

There are no such residues in this entry.