



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:41 PM GMT

PDB ID : 2GD1  
Title : COENZYME-INDUCED CONFORMATIONAL CHANGES IN GLYCER  
ALDEHYDE-3-PHOSPHATEDEHYDROGENASE FROM BACILLUS  
STEAROTHERMOPHILLUS  
Authors : Skarzynski, T.; Wonacott, A.J.  
Deposited on : 1989-06-29  
Resolution : 2.50 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>

---

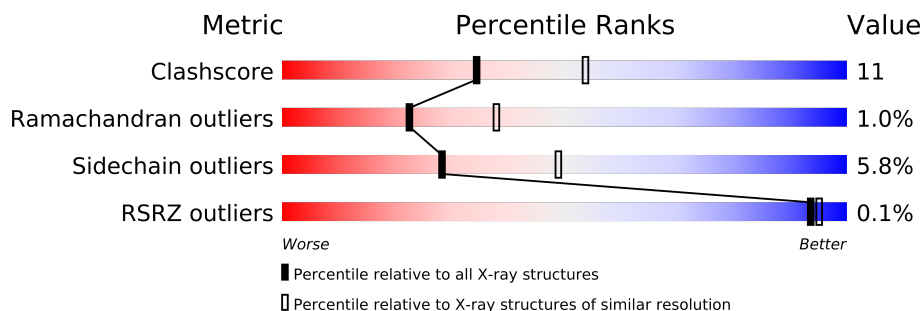
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 3 unique types of molecules in this entry. The entry contains 10644 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 APO-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		

*Continued on next page...*

*Continued from previous page...*

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.

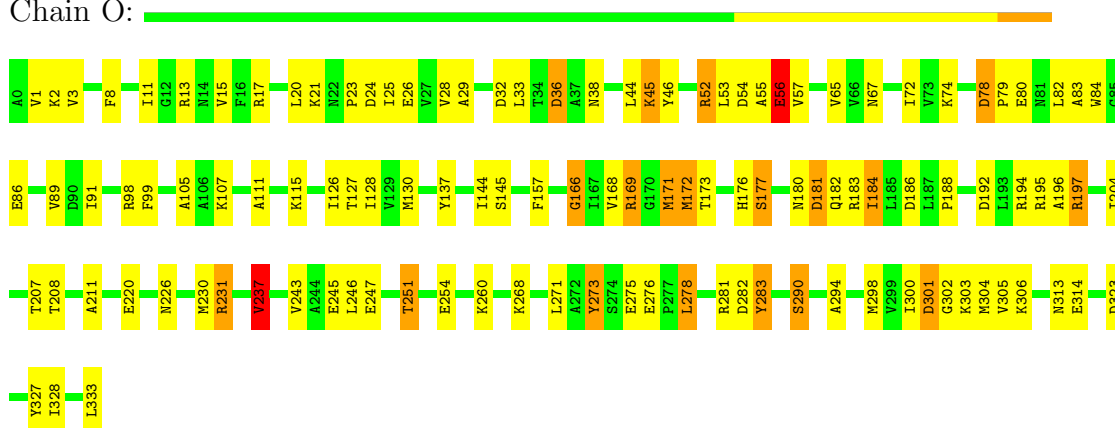
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	114	Total	O	0	0
			114	114		
3	P	127	Total	O	0	0
			127	127		
3	Q	121	Total	O	0	0
			121	121		
3	R	142	Total	O	0	0
			142	142		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

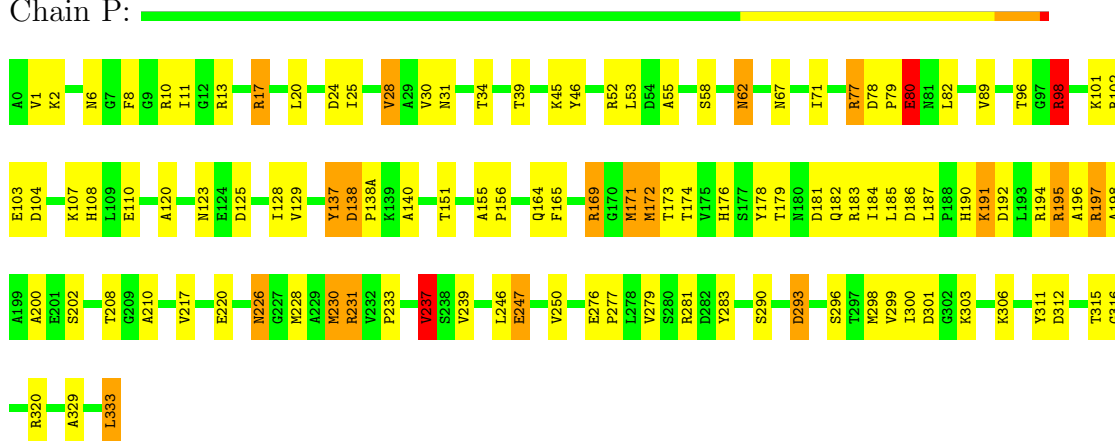
#### • Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

Chain O:



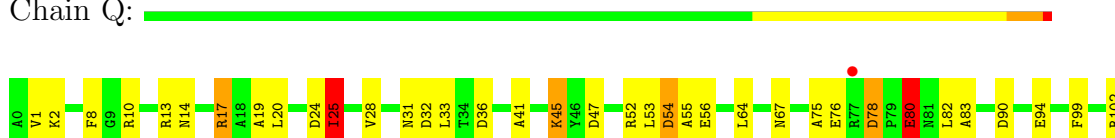
#### • Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

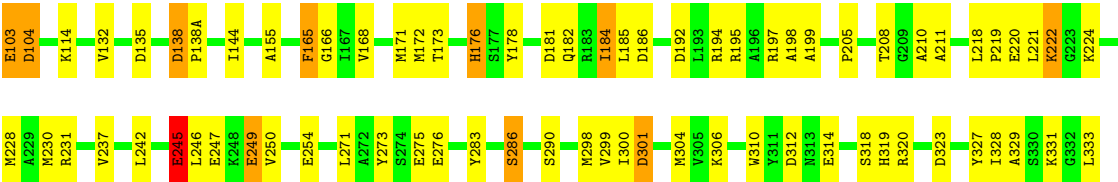
Chain P:



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

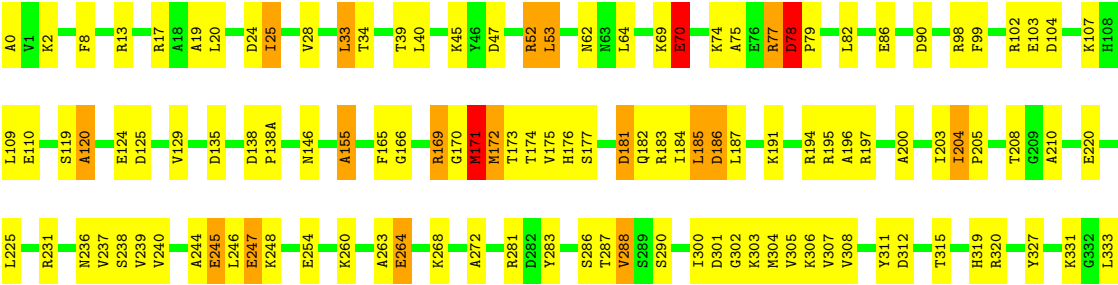
Chain Q:





● Molecule 1: APO-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, $\alpha$ , $\beta$ , $\gamma$	83.80Å 129.20Å 83.10Å 90.00° 107.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 24.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 94.9 (24.73-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 2.50Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.177 , (Not available) 0.166 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.7	EDS
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 55743 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.98	0/2561	1.80	53/3474 (1.5%)
1	P	1.02	0/2561	1.90	56/3474 (1.6%)
1	Q	1.00	0/2561	1.84	52/3474 (1.5%)
1	R	1.01	0/2561	1.94	64/3474 (1.8%)
All	All	1.00	0/10244	1.87	225/13896 (1.6%)

There are no bond length outliers.

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	197	ARG	NE-CZ-NH1	21.38	130.99	120.30
1	O	197	ARG	NE-CZ-NH2	17.40	129.00	120.30
1	R	181	ASP	CB-CG-OD1	14.28	131.15	118.30
1	R	194	ARG	CD-NE-CZ	13.39	142.34	123.60
1	O	194	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	R	171	MET	CA-CB-CG	12.54	134.62	113.30
1	R	125	ASP	CB-CG-OD1	12.44	129.50	118.30
1	Q	78	ASP	CB-CG-OD1	12.18	129.26	118.30
1	R	197	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	R	320	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	R	169	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	O	183	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	R	320	ARG	CD-NE-CZ	11.35	139.49	123.60
1	P	197	ARG	NE-CZ-NH2	-10.95	114.82	120.30
1	Q	13	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	O	183	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	P	320	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	P	231	ARG	NE-CZ-NH2	10.45	125.52	120.30
1	Q	102	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	Q	276	GLU	OE1-CD-OE2	10.28	135.63	123.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	98	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	P	281	ARG	CD-NE-CZ	9.94	137.52	123.60
1	P	17	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	P	138	ASP	CB-CG-OD1	9.60	126.94	118.30
1	P	195	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	Q	186	ASP	CB-CG-OD1	9.50	126.85	118.30
1	P	171	MET	CA-CB-CG	9.45	129.37	113.30
1	O	197	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	R	13	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	R	135	ASP	CB-CG-OD1	9.27	126.64	118.30
1	P	281	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	Q	194	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	Q	312	ASP	CB-CG-OD1	9.02	126.41	118.30
1	Q	301	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	P	24	ASP	CB-CG-OD1	8.87	126.28	118.30
1	Q	320	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	P	231	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	O	301	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	P	24	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	O	98	ARG	CD-NE-CZ	8.50	135.50	123.60
1	P	137	TYR	CB-CG-CD1	8.39	126.03	121.00
1	R	47	ASP	CB-CG-OD1	8.24	125.72	118.30
1	P	102	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	Q	17	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	P	138	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	P	125	ASP	CB-CG-OD1	8.01	125.51	118.30
1	Q	186	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	P	77	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	P	191	LYS	CA-CB-CG	7.90	130.79	113.40
1	P	293	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	Q	192	ASP	CB-CG-OD1	7.86	125.38	118.30
1	Q	24	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	Q	245	GLU	CA-CB-CG	7.78	130.52	113.40
1	R	281	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	O	194	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	R	247	GLU	CA-CB-CG	7.66	130.25	113.40
1	Q	135	ASP	CB-CG-OD1	7.56	125.11	118.30
1	O	13	ARG	CD-NE-CZ	7.55	134.18	123.60
1	O	98	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	R	181	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	O	13	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	Q	197	ARG	NE-CZ-NH1	7.41	124.00	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	70	GLU	CA-CB-CG	7.31	129.49	113.40
1	R	102	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	R	186	ASP	CB-CG-OD1	7.29	124.87	118.30
1	R	17	ARG	CD-NE-CZ	7.28	133.79	123.60
1	R	125	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	R	90	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	R	102	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	R	90	ASP	CB-CG-OD1	7.17	124.75	118.30
1	R	171	MET	CG-SD-CE	7.15	111.64	100.20
1	Q	323	ASP	CB-CG-OD1	7.15	124.73	118.30
1	Q	192	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	R	124	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	R	245	GLU	CA-CB-CG	6.99	128.77	113.40
1	Q	155	ALA	CB-CA-C	6.98	120.58	110.10
1	R	13	ARG	NH1-CZ-NH2	-6.89	111.82	119.40
1	P	183	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	Q	102	ARG	CD-NE-CZ	-6.83	114.03	123.60
1	P	231	ARG	CD-NE-CZ	6.79	133.10	123.60
1	R	77	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	R	173	THR	N-CA-CB	6.74	123.10	110.30
1	Q	32	ASP	CB-CG-OD1	6.73	124.35	118.30
1	R	110	GLU	CG-CD-OE1	6.72	131.75	118.30
1	O	33	LEU	CA-CB-CG	6.72	130.75	115.30
1	O	111	ALA	N-CA-CB	6.72	119.50	110.10
1	Q	80	GLU	CA-CB-CG	6.67	128.09	113.40
1	O	52	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	R	254	GLU	CA-CB-CG	6.57	127.86	113.40
1	O	273	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	P	46	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	P	194	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	R	194	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	Q	320	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	O	220	GLU	CA-CB-CG	6.51	127.72	113.40
1	P	110	GLU	CG-CD-OE2	-6.51	105.29	118.30
1	Q	54	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	Q	327	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	R	52	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	R	272	ALA	CB-CA-C	6.40	119.70	110.10
1	O	323	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	R	186	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	R	78	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	Q	194	ARG	CD-NE-CZ	6.29	132.41	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	33	LEU	CA-CB-CG	6.29	129.76	115.30
1	P	52	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	Q	36	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	O	54	ASP	CB-CG-OD1	6.21	123.89	118.30
1	R	155	ALA	CB-CA-C	6.21	119.42	110.10
1	O	8	PHE	CB-CG-CD2	-6.21	116.46	120.80
1	P	226	ASN	CB-CA-C	6.20	122.80	110.40
1	Q	194	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	O	192	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	P	17	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	O	78	ASP	CB-CG-OD1	6.17	123.85	118.30
1	O	177	SER	CA-CB-OG	-6.16	94.56	111.20
1	P	169	ARG	CD-NE-CZ	6.16	132.22	123.60
1	P	55	ALA	N-CA-CB	6.15	118.71	110.10
1	Q	247	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	O	245	GLU	CA-CB-CG	6.12	126.86	113.40
1	Q	254	GLU	CA-CB-CG	6.12	126.86	113.40
1	O	273	TYR	CB-CG-CD1	6.10	124.66	121.00
1	P	290	SER	CA-CB-OG	6.08	127.60	111.20
1	P	298	MET	CA-CB-CG	6.07	123.63	113.30
1	O	231	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	O	173	THR	N-CA-CB	6.07	121.82	110.30
1	R	40	LEU	CA-CB-CG	6.04	129.20	115.30
1	R	264	GLU	OE1-CD-OE2	6.03	130.53	123.30
1	P	123	ASN	OD1-CG-ND2	6.03	135.76	121.90
1	O	17	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	O	169	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	O	130	MET	CB-CA-C	5.99	122.38	110.40
1	P	320	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	P	125	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	Q	75	ALA	CB-CA-C	5.96	119.04	110.10
1	R	75	ALA	CB-CA-C	5.96	119.03	110.10
1	R	78	ASP	CA-CB-CG	-5.90	100.43	113.40
1	R	200	ALA	C-N-CA	5.87	136.38	121.70
1	R	288	VAL	CA-CB-CG1	5.82	119.63	110.90
1	Q	320	ARG	CD-NE-CZ	5.81	131.73	123.60
1	R	13	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	R	204	ILE	CA-CB-CG1	-5.77	100.05	111.00
1	Q	199	ALA	CB-CA-C	-5.76	101.46	110.10
1	O	278	LEU	CB-CA-C	5.75	121.14	110.20
1	P	10	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	Q	173	THR	CA-CB-CG2	5.71	120.39	112.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	80	GLU	CG-CD-OE1	5.70	129.70	118.30
1	P	98	ARG	CD-NE-CZ	5.70	131.58	123.60
1	P	171	MET	N-CA-CB	-5.69	100.35	110.60
1	O	36	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	P	299	VAL	CG1-CB-CG2	-5.65	101.87	110.90
1	P	191	LYS	N-CA-CB	5.63	120.74	110.60
1	P	96	THR	N-CA-CB	5.63	121.00	110.30
1	R	203	ILE	C-N-CA	5.63	135.78	121.70
1	R	69	LYS	CB-CA-C	-5.62	99.17	110.40
1	Q	47	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	P	62	ASN	O-C-N	5.61	131.68	122.70
1	Q	298	MET	CG-SD-CE	-5.61	91.22	100.20
1	O	313	ASN	O-C-N	-5.60	113.75	122.70
1	P	228	MET	CA-CB-CG	-5.58	103.81	113.30
1	P	239	VAL	CA-CB-CG1	5.57	119.25	110.90
1	R	17	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	P	192	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	O	32	ASP	CB-CG-OD1	5.50	123.25	118.30
1	Q	102	ARG	C-N-CA	5.48	135.40	121.70
1	P	237	VAL	CA-CB-CG1	5.48	119.11	110.90
1	O	207	THR	CA-CB-OG1	-5.45	97.55	109.00
1	R	138	ASP	CB-CG-OD1	5.45	123.21	118.30
1	O	226	ASN	N-CA-CB	5.45	120.41	110.60
1	P	173	THR	N-CA-CB	5.45	120.65	110.30
1	P	58	SER	N-CA-CB	5.45	118.67	110.50
1	P	80	GLU	CA-CB-CG	5.43	125.35	113.40
1	O	194	ARG	CD-NE-CZ	5.42	131.19	123.60
1	Q	230	MET	O-C-N	5.41	131.36	122.70
1	P	140	ALA	N-CA-CB	-5.41	102.53	110.10
1	Q	104	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	O	251	THR	N-CA-CB	5.39	120.54	110.30
1	R	194	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	O	314	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	R	327	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	R	109	LEU	CB-CA-C	5.35	120.37	110.20
1	Q	25	ILE	N-CA-CB	5.34	123.08	110.80
1	Q	176	HIS	N-CA-CB	-5.34	100.99	110.60
1	O	303	LYS	N-CA-C	5.33	125.39	111.00
1	Q	24	ASP	OD1-CG-OD2	5.33	133.42	123.30
1	R	86	GLU	OE1-CD-OE2	5.31	129.67	123.30
1	P	312	ASP	CB-CG-OD1	5.29	123.07	118.30
1	O	282	ASP	CB-CG-OD1	5.29	123.06	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	283	TYR	CA-CB-CG	-5.29	103.35	113.40
1	O	237	VAL	CA-CB-CG2	5.28	118.82	110.90
1	P	13	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	R	62	ASN	N-CA-CB	5.27	120.08	110.60
1	R	98	ARG	CD-NE-CZ	5.26	130.96	123.60
1	Q	138	ASP	CB-CG-OD1	5.24	123.02	118.30
1	Q	103	GLU	CA-CB-CG	5.22	124.88	113.40
1	R	175	VAL	CA-CB-CG1	5.20	118.70	110.90
1	P	230	MET	N-CA-CB	5.19	119.93	110.60
1	R	174	THR	O-C-N	5.18	131.00	122.70
1	R	239	VAL	CA-CB-CG2	5.18	118.67	110.90
1	R	231	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	P	312	ASP	N-CA-C	-5.15	97.09	111.00
1	R	78	ASP	OD1-CG-OD2	5.15	133.08	123.30
1	O	231	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	O	230	MET	CG-SD-CE	5.14	108.42	100.20
1	O	327	TYR	CB-CG-CD2	5.13	124.08	121.00
1	O	157	PHE	CB-CA-C	5.12	120.63	110.40
1	Q	197	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	R	53	LEU	CB-CA-C	5.11	119.91	110.20
1	P	11	ILE	CA-C-O	-5.10	109.39	120.10
1	P	197	ARG	CG-CD-NE	-5.10	101.09	111.80
1	O	166	GLY	O-C-N	5.09	130.84	122.70
1	Q	249	GLU	N-CA-CB	5.08	119.74	110.60
1	O	181	ASP	N-CA-CB	-5.07	101.48	110.60
1	Q	103	GLU	CB-CG-CD	5.06	127.85	114.20
1	Q	80	GLU	CB-CG-CD	5.05	127.85	114.20
1	R	185	LEU	CB-CA-C	5.05	119.79	110.20
1	R	183	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	Q	301	ASP	CB-CG-OD1	5.04	122.84	118.30
1	Q	210	ALA	CB-CA-C	5.04	117.66	110.10
1	R	231	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	O	130	MET	CG-SD-CE	-5.03	92.16	100.20
1	O	56	GLU	N-CA-CB	5.03	119.64	110.60
1	Q	94	GLU	CG-CD-OE2	-5.01	108.27	118.30
1	O	177	SER	N-CA-CB	-5.00	102.99	110.50
1	O	327	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	66	0
1	P	2525	0	2572	62	0
1	Q	2525	0	2572	61	0
1	R	2525	0	2572	57	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	6	0
3	P	127	0	0	3	0
3	Q	121	0	0	7	0
3	R	142	0	0	6	0
All	All	10644	0	10288	221	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 11.

All (221) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:O:304:MET:HG2	1:P:171:MET:HE2	1.76	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:Q:78:ASP:OD1	1:Q:80:GLU:HB2	1.97	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: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:R:186:ASP:HA	1:R:196:ALA:O	2.02	0.59
1:Q:211:ALA:HB3	3:Q:352:HOH:O	2.02	0.59
1:P:237:VAL:HG11	1:P:283:TYR:HB2	1.84	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:HE2	1:R:304:MET:HG2	1.86	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:P:186:ASP:HB2	1:Q:10:ARG:HH12	1.71	0.56
1:O:115:LYS:HE3	1:O:137:TYR:OH	2.06	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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:O:237:VAL:HG11	1:O:283:TYR:HB2	1.89	0.53
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: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:O:211:ALA:HB3	3:O:343:HOH:O	2.08	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:Q:19:ALA:HB1	1:Q:25:ILE:HD11	1.90	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:O:36:ASP:OD1	1:O:38:ASN:HB2	2.11	0.51
1:O:304:MET:HG2	1:P:171:MET:HE3	1.90	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:Q:41:ALA:HB2	1:Q:64:LEU:CD2	2.43	0.49
1:P:78:ASP:OD2	1:P:80:GLU:HB2	2.12	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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:20:LEU:HD11	1:O:53:LEU:HD11	1.94	0.49
1:Q:82:LEU:O	1:Q:83:ALA:C	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:O:45:LYS:HB3	1:O:46:TYR:CD2	2.48	0.49
1:R:181:ASP:OD1	1:R:195:ARG:HD3	2.13	0.49
1:R:181:ASP:OD1	1:R:195:ARG:NH1	2.44	0.48
1:O:182:GLN:HB3	3:O:357:HOH:O	2.11	0.48
1:P:172:MET:HE2	1:P:208:THR:HG21	1.94	0.48
1:Q:144:ILE:HD13	1:Q:328:ILE:CD1	2.37	0.48
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:P:186:ASP:HA	1:P:196:ALA:O	2.13	0.48
1:O:243:VAL:HA	1:O:305:VAL:O	2.14	0.48
1:R:99:PHE:HD1	1:R:104:ASP:HB3	1.78	0.48
1:R:20:LEU:HD12	1:R:53:LEU:HD11	1.96	0.48
1:Q:271:LEU:HD12	1:Q:290:SER:HB3	1.94	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:P:172:MET:CE	1:P:208:THR:HG21	2.45	0.47
1:P:315:THR:O	1:P:316:GLY:C	2.53	0.47
1:Q:14:ASN:HB3	1:Q:318:SER:OG	2.15	0.47
1:R:119:SER:O	1:R:120:ALA:HB2	2.15	0.46
1:O:281:ARG:HG2	1:P:202:SER:OG	2.15	0.46
1:P:129:VAL:CG2	1:P:217:VAL:HG11	2.43	0.46
1:O:276:GLU:HB2	1:O:278:LEU:HG	1.96	0.46
1:P:151:THR:OG1	1:P:210:ALA:HA	2.14	0.46
1:P:155:ALA:HB3	1:P:156:PRO:HD3	1.98	0.46
1:O:301:ASP:HB2	1:P:169:ARG:CD	2.46	0.46
1:R:34:THR:HG22	1:R:39:THR:HB	1.97	0.46
1:O:3:VAL:HA	1:O:91:ILE:O	2.15	0.46
1:O:300:ILE:HD11	1:P:226:ASN:CB	2.45	0.46
1:P:172:MET:HE1	1:P:174:THR:HB	1.96	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:R:204:ILE:HA	1:R:205:PRO:HD3	1.82	0.45
1:O:21:LYS:NZ	3:O:419:HOH:O	2.46	0.45
1:R:129:VAL:HG11	1:R:155:ALA:HB3	1.99	0.45
1:Q:328:ILE:HD13	1:Q:328:ILE:HG21	1.80	0.44
1:O:273:TYR:CE1	1:O:294:ALA:HB2	2.52	0.44
1:R:236:ASN:ND2	1:R:312:ASP:OD2	2.43	0.44
1:O:74:LYS:HE3	1:O:82:LEU:O	2.18	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: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:R:172:MET:HE1	1:R:208:THR:HG21	1.99	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: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:HH21	1:P:231:ARG:HG3	1.83	0.43
1:O:180:ASN:HB2	1:R:187:LEU:HD11	2.00	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:R:172:MET:CE	1:R:208:THR:HG21	2.49	0.42
1:R:263:ALA:O	1:R:268:LYS:HA	2.19	0.42
1:P:128:ILE:HD11	1:P:137:TYR:HB2	2.00	0.42
1:R:19:ALA:CB	1:R:25:ILE:HD11	2.49	0.42
1:R:20:LEU:HD23	1:R:20:LEU:HA	1.76	0.42
1:P:329:ALA:HA	1:P:333:LEU:HD22	2.02	0.42
1:P:20:LEU:HD12	1:P:53:LEU:HD11	2.02	0.42
1:O:275:GLU:HB2	3:O:391:HOH:O	2.18	0.42
1:O:281:ARG:NH1	3:O:434:HOH:O	2.32	0.42
1:Q:138:ASP:HA	1:Q:138(A):PRO:HD2	1.83	0.42
1:P:104:ASP:O	1:P:107:LYS:HG3	2.20	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:82:LEU:O	1:O:83:ALA:C	2.57	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
1:Q:41:ALA:O	1:Q:45:LYS:HB2	2.20	0.42
1:Q:31:ASN:CG	1:Q:82:LEU:HD21	2.40	0.42
1:O:184:ILE:HG21	1:O:184:ILE:HD13	1.81	0.42
1:P:138:ASP:HA	1:P:138(A):PRO:HD2	1.92	0.42
1:O:83:ALA:HB1	1:O:86:GLU:HG3	2.02	0.41
1:O:29:ALA:HA	1:O:72:ILE:O	2.20	0.41
1:Q:171:MET:HG3	1:R:306:LYS:HE2	2.02	0.41
1:P:333:LEU:HA	1:P:333:LEU:HD12	1.93	0.41
1:R:220:GLU:HG3	3:R:470:HOH:O	2.19	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:P:176:HIS:HB3	1:P:231:ARG:HD3	2.01	0.41
1:R:244:ALA:O	1:R:305:VAL:HG12	2.20	0.41
1:Q:301:ASP:HB2	1:R:169:ARG:CD	2.50	0.41
1:Q:54:ASP:O	1:Q:55:ALA:HB2	2.21	0.41
1:Q:20:LEU:HD12	1:Q:53:LEU:HD11	2.03	0.41
1:O:99:PHE:O	1:O:105:ALA:HB2	2.20	0.41
1:Q:1:VAL:HG21	1:Q:329:ALA:HB2	2.02	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:165:PHE:CD2	1:Q:250:VAL:HG11	2.56	0.41
1:R:286:SER:O	1:R:315:THR:HB	2.21	0.41
1:R:172:MET:HE2	1:R:210:ALA:HB3	2.03	0.41
1:Q:205:PRO:HB3	1:Q:228:MET:CE	2.51	0.41
1:O:56:GLU:H	1:O:67:ASN:HD21	1.67	0.40
1:O:84:TRP:CE3	1:O:89:VAL:HG11	2.55	0.40
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.56	0.40
1:Q:300:ILE:HD13	1:Q:300:ILE:HG21	1.75	0.40
1:Q:314:GLU:HG2	3:Q:438:HOH:O	2.21	0.40
1:P:300:ILE:HD13	1:P:300:ILE:HG21	1.86	0.40
1:P:1:VAL:HG21	1:P:329:ALA:HB2	2.03	0.40
1:Q:17:ARG:HH11	1:Q:17:ARG:HD3	1.50	0.40
1:O:126:ILE:HG12	1:O:128:ILE:HG13	2.04	0.40
1:R:184:ILE:HG22	1:R:185:LEU:HG	2.04	0.40
1:P:247:GLU:O	1:P:303:LYS:HE2	2.22	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%)	309 (93%)	20 (6%)	3 (1%)	25	42
1	P	332/334 (99%)	314 (95%)	15 (4%)	3 (1%)	25	42
1	Q	332/334 (99%)	319 (96%)	10 (3%)	3 (1%)	25	42
1	R	332/334 (99%)	311 (94%)	17 (5%)	4 (1%)	19	32
All	All	1328/1336 (99%)	1253 (94%)	62 (5%)	13 (1%)	22	38

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 ⓘ

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%)	259 (95%)	13 (5%)	35	60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	272/272 (100%)	254 (93%)	18 (7%)	24	41
1	Q	272/272 (100%)	256 (94%)	16 (6%)	28	48
1	R	272/272 (100%)	256 (94%)	16 (6%)	28	48
All	All	1088/1088 (100%)	1025 (94%)	63 (6%)	28	49

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	23	PRO
1	O	25	ILE
1	O	45	LYS
1	O	52	ARG
1	O	56	GLU
1	O	171	MET
1	O	172	MET
1	O	177	SER
1	O	184	ILE
1	O	246	LEU
1	O	268	LYS
1	O	290	SER
1	O	333	LEU
1	P	2	LYS
1	P	8	PHE
1	P	25	ILE
1	P	28	VAL
1	P	30	VAL
1	P	45	LYS
1	P	62	ASN
1	P	71	ILE
1	P	77	ARG
1	P	80	GLU
1	P	98	ARG
1	P	164	GLN
1	P	172	MET
1	P	230	MET
1	P	246	LEU
1	P	247	GLU
1	P	311	TYR
1	P	333	LEU
1	Q	8	PHE
1	Q	25	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	33	LEU
1	Q	45	LYS
1	Q	80	GLU
1	Q	103	GLU
1	Q	165	PHE
1	Q	184	ILE
1	Q	220	GLU
1	Q	222	LYS
1	Q	245	GLU
1	Q	246	LEU
1	Q	249	GLU
1	Q	275	GLU
1	Q	286	SER
1	Q	333	LEU
1	R	8	PHE
1	R	25	ILE
1	R	33	LEU
1	R	70	GLU
1	R	74	LYS
1	R	77	ARG
1	R	78	ASP
1	R	171	MET
1	R	172	MET
1	R	191	LYS
1	R	245	GLU
1	R	247	GLU
1	R	300	ILE
1	R	301	ASP
1	R	311	TYR
1	R	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	62	ASN
1	O	67	ASN
1	O	81	ASN
1	P	67	ASN
1	P	81	ASN
1	Q	62	ASN
1	Q	67	ASN
1	Q	81	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	146	ASN
1	Q	319	HIS
1	R	67	ASN
1	R	81	ASN
1	R	146	ASN

### 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 ⓘ

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	O	338	-	4,4,4	1.15	0	6,6,6	0.23	0
2	SO4	O	339	-	4,4,4	1.15	0	6,6,6	0.50	0
2	SO4	P	338	-	4,4,4	1.18	0	6,6,6	0.26	0
2	SO4	P	339	-	4,4,4	1.15	0	6,6,6	0.35	0
2	SO4	Q	338	-	4,4,4	1.01	0	6,6,6	0.47	0
2	SO4	Q	339	-	4,4,4	1.00	0	6,6,6	0.24	0
2	SO4	R	338	-	4,4,4	1.07	0	6,6,6	0.45	0
2	SO4	R	339	-	4,4,4	1.00	0	6,6,6	0.21	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
2	SO4	O	338	-	-	0/0/0/0	0/0/0/0
2	SO4	O	339	-	-	0/0/0/0	0/0/0/0
2	SO4	P	338	-	-	0/0/0/0	0/0/0/0
2	SO4	P	339	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	338	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	339	-	-	0/0/0/0	0/0/0/0
2	SO4	R	338	-	-	0/0/0/0	0/0/0/0
2	SO4	R	339	-	-	0/0/0/0	0/0/0/0

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.

## 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%)	-0.45	0 100 100	5, 16, 38, 55	0
1	P	334/334 (100%)	-0.48	0 100 100	4, 15, 38, 59	0
1	Q	334/334 (100%)	-0.49	1 (0%) 91 93	3, 16, 40, 55	0
1	R	334/334 (100%)	-0.46	0 100 100	3, 15, 36, 51	0
All	All	1336/1336 (100%)	-0.47	1 (0%) 93 95	3, 16, 38, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	77	ARG	2.3

### 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	R	338	5/5	0.29	-	37,37,37,38	5
2	SO4	Q	338	5/5	0.25	-	35,36,36,36	5
2	SO4	P	339	5/5	0.32	-	35,36,37,37	5
2	SO4	R	339	5/5	0.25	-	30,30,32,32	5
2	SO4	Q	339	5/5	0.27	-	33,33,33,35	5
2	SO4	O	338	5/5	0.28	-	32,32,33,34	5
2	SO4	O	339	5/5	0.25	-	32,33,33,33	5
2	SO4	P	338	5/5	0.20	-	32,33,34,35	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.