



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:25 AM UTC

PDB ID : 1OBF / pdb_00001obf
Title : The crystal structure of Glyceraldehyde 3-phosphate Dehydrogenase from *Alcaligenes xylosoxidans* at 1.7Å resolution.
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Deposited on : 2003-01-30
Resolution : 1.70 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

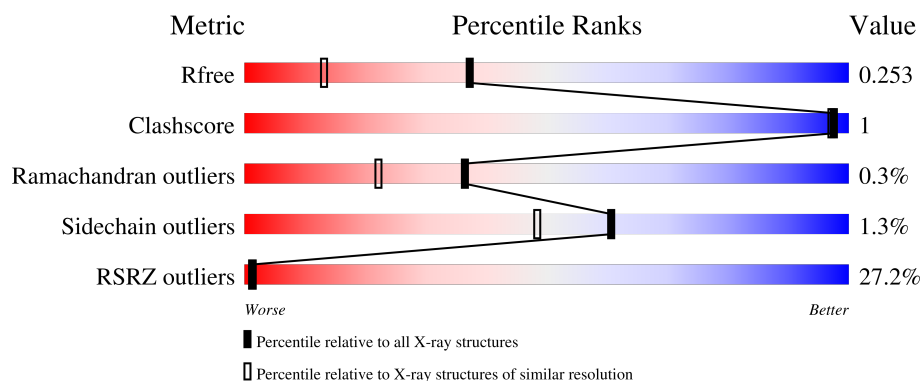
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	335	7% 97%
1	P	335	47% 96%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5563 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 GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	335	Total	C	N	O	S	0	1	0
			2516	1569	443	495	9			
1	P	335	Total	C	N	O	S	0	1	0
			2516	1569	443	495	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

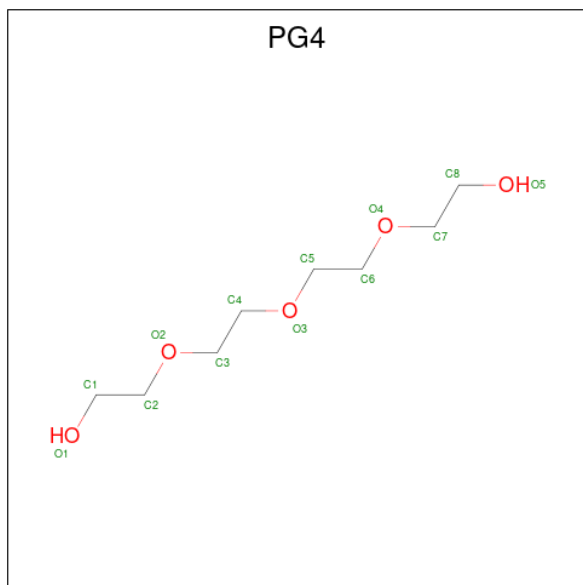


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total K 1 1	0	0
3	P	1	Total K 1 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total C O 13 8 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	247	Total O 247 247	0	0
5	P	254	Total O 254 254	0	0

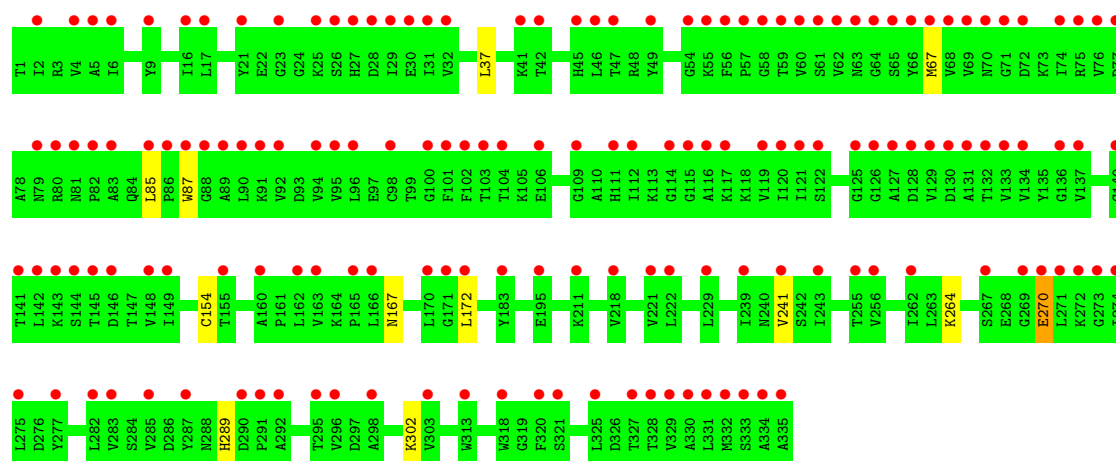
3 Residue-property plots

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: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE



• Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.98Å 146.62Å 146.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-1.70) 97.0 (50.00-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.06 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.166 , 0.187 0.242 , 0.253	Depositor DCC
R_{free} test set	5107 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5563	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PG4, K, CSD

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	0.89	0/2550	0.91	0/3470
1	P	0.87	1/2550 (0.0%)	0.89	0/3470
All	All	0.88	1/5100 (0.0%)	0.90	0/6940

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	67	MET	SD-CE	-5.10	1.66	1.79

There are no bond angle outliers.

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	2516	0	2519	2	0
1	P	2516	0	2519	5	0
2	O	10	0	0	0	0
2	P	5	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	P	13	0	18	1	0
5	O	247	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	254	0	0	2	1
All	All	5563	0	5056	8	1

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 1.

All (8) 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)
4:P:344:PG4:O5	5:P:2254:HOH:O	2.00	0.80
1:P:167:ASN:HD22	1:P:172:LEU:H	1.50	0.60
5:O:2164:HOH:O	1:P:302:LYS:HE3	2.12	0.50
1:P:85:LEU:HD13	1:P:87:TRP:CZ2	2.49	0.48
1:O:85:LEU:HD13	1:O:87:TRP:CZ2	2.51	0.46
1:P:264:LYS:NZ	5:P:2188:HOH:O	2.51	0.44
1:P:270:GLU:CD	1:P:270:GLU:H	2.26	0.43
1:O:212:THR:HG22	1:O:232:TYR:HA	2.04	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:2174:HOH:O	5:P:2233:HOH:O[3_655]	2.14	0.06

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	332/335 (99%)	325 (98%)	6 (2%)	1 (0%)	36	22
1	P	332/335 (99%)	323 (97%)	8 (2%)	1 (0%)	36	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	664/670 (99%)	648 (98%)	14 (2%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	241	VAL
1	P	241	VAL

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%)	268 (98%)	4 (2%)	57	43
1	P	272/272 (100%)	269 (99%)	3 (1%)	65	54
All	All	544/544 (100%)	537 (99%)	7 (1%)	61	48

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	61	SER
1	O	106	GLU
1	O	162	LEU
1	O	270	GLU
1	P	37	LEU
1	P	270	GLU
1	P	289	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	260	ASN
1	P	167	ASN
1	P	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CSD	P	154[B]	-	4,7,8	15.19	1 (25%)	1,8,10	3.97	1 (100%)
1	CSD	O	154[A]	-	4,7,8	12.96	1 (25%)	1,8,10	0.73	0
1	CSD	P	154[A]	-	4,7,8	15.19	1 (25%)	1,8,10	3.97	1 (100%)
1	CSD	O	154[B]	-	4,7,8	12.96	1 (25%)	1,8,10	0.73	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
1	CSD	P	154[B]	-	-	1/2/6/8	-
1	CSD	O	154[A]	-	-	0/2/6/8	-
1	CSD	P	154[A]	-	-	1/2/6/8	-
1	CSD	O	154[B]	-	-	0/2/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	154[A]	CSD	OD1-SG	30.35	1.75	1.47
1	P	154[B]	CSD	OD1-SG	30.35	1.75	1.47
1	O	154[A]	CSD	OD1-SG	25.88	1.71	1.47
1	O	154[B]	CSD	OD1-SG	25.88	1.71	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	154[A]	CSD	OD1-SG-CB	3.97	112.92	105.60
1	P	154[B]	CSD	OD1-SG-CB	3.97	112.92	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	154[A]	CSD	CA-CB-SG-OD1
1	P	154[B]	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	O	342	-	4,4,4	0.18	0	6,6,6	0.46	0
2	SO4	O	341	-	4,4,4	0.25	0	6,6,6	0.19	0
4	PG4	P	344	3	12,12,12	0.57	0	11,11,11	0.23	0
2	SO4	P	341	-	4,4,4	0.31	0	6,6,6	0.16	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
4	PG4	P	344	3	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	344	PG4	O2-C3-C4-O3
4	P	344	PG4	C1-C2-O2-C3
4	P	344	PG4	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	344	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/335 (99%)	0.91	25 (7%)	20 22	16, 24, 36, 42	1 (0%)
1	P	334/335 (99%)	2.05	157 (47%)	0 0	16, 25, 40, 46	1 (0%)
All	All	668/670 (99%)	1.48	182 (27%)	1 1	16, 25, 38, 46	2 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	66	TYR	5.0
1	P	335	ALA	4.8
1	P	65	SER	4.7
1	P	60	VAL	4.7
1	P	76	VAL	4.6
1	P	101	PHE	4.6
1	P	68	VAL	4.5
1	P	112	ILE	4.4
1	P	87	TRP	4.3
1	P	90	LEU	4.1
1	P	116	ALA	4.1
1	P	334	ALA	4.0
1	P	145	THR	3.9
1	P	32	VAL	3.9
1	P	277	TYR	3.9
1	P	95	VAL	3.8
1	P	325	LEU	3.8
1	P	127	ALA	3.8
1	P	62	VAL	3.8
1	P	80	ARG	3.8
1	O	126	GLY	3.8
1	P	328	THR	3.8
1	P	31	ILE	3.7
1	P	61	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	P	74	ILE	3.6
1	P	121	ILE	3.6
1	P	89	ALA	3.6
1	P	56	PHE	3.5
1	P	4	VAL	3.5
1	P	131	ALA	3.5
1	P	69	VAL	3.5
1	P	92	VAL	3.5
1	P	2	ILE	3.5
1	P	58	GLY	3.5
1	P	102	PHE	3.4
1	P	287	TYR	3.4
1	P	149	ILE	3.4
1	P	146	ASP	3.4
1	P	269	GLY	3.4
1	P	292	ALA	3.3
1	P	59	THR	3.3
1	P	94	VAL	3.3
1	P	270	GLU	3.3
1	O	335	ALA	3.3
1	P	330	ALA	3.3
1	P	81	ASN	3.3
1	P	49	TYR	3.2
1	P	57	PRO	3.2
1	P	282	LEU	3.2
1	O	127	ALA	3.2
1	O	80	ARG	3.2
1	P	85	LEU	3.2
1	P	125	GLY	3.1
1	P	27	HIS	3.1
1	P	83	ALA	3.1
1	P	148	VAL	3.1
1	P	111	HIS	3.1
1	P	64	GLY	3.1
1	P	262	ILE	3.1
1	P	96	LEU	3.1
1	P	70	ASN	3.1
1	O	195	GLU	3.0
1	P	320	PHE	3.0
1	P	141	THR	3.0
1	P	142	LEU	3.0
1	P	26	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	163	VAL	2.9
1	P	25	LYS	2.9
1	P	331	LEU	2.9
1	P	329	VAL	2.9
1	P	313	TRP	2.9
1	P	103	THR	2.8
1	O	221	VAL	2.8
1	P	129	VAL	2.8
1	P	72	ASP	2.8
1	P	136	GLY	2.8
1	P	21	TYR	2.8
1	P	295	THR	2.8
1	O	192	VAL	2.8
1	P	133	VAL	2.8
1	O	232	TYR	2.8
1	P	100	GLY	2.8
1	P	46	LEU	2.7
1	P	166	LEU	2.7
1	P	75	ARG	2.7
1	O	89	ALA	2.7
1	O	334	ALA	2.7
1	P	82	PRO	2.7
1	P	296	VAL	2.7
1	P	211	LYS	2.7
1	O	214	ALA	2.7
1	P	98	CYS	2.6
1	O	62	VAL	2.6
1	P	9	TYR	2.6
1	P	318	TRP	2.6
1	P	29	ILE	2.6
1	P	332	MET	2.6
1	P	222	LEU	2.6
1	P	239	ILE	2.6
1	O	101	PHE	2.6
1	P	275	LEU	2.6
1	P	6	ILE	2.6
1	P	298	ALA	2.6
1	P	86	PRO	2.6
1	P	106	GLU	2.6
1	P	114	GLY	2.5
1	P	144	SER	2.5
1	P	271	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	333	SER	2.5
1	O	217	ALA	2.5
1	P	255	THR	2.5
1	P	229	LEU	2.5
1	P	283	VAL	2.5
1	P	109	GLY	2.5
1	P	273	GLY	2.5
1	P	42	THR	2.5
1	P	267	SER	2.5
1	P	17	LEU	2.5
1	P	5	ALA	2.5
1	P	143	LYS	2.4
1	P	165	PRO	2.4
1	O	83	ALA	2.4
1	P	241	VAL	2.4
1	P	327	THR	2.4
1	P	79	ASN	2.4
1	P	54	GLY	2.4
1	P	28	ASP	2.4
1	P	291	PRO	2.4
1	P	120	ILE	2.4
1	P	243	ILE	2.4
1	P	122	SER	2.3
1	P	126	GLY	2.3
1	O	307	LEU	2.3
1	P	162	LEU	2.3
1	P	140	GLY	2.3
1	P	290	ASP	2.3
1	P	195	GLU	2.3
1	P	321	SER	2.3
1	P	256	VAL	2.3
1	P	47	THR	2.3
1	P	104	THR	2.3
1	O	85	LEU	2.3
1	P	183	TYR	2.3
1	P	130	ASP	2.3
1	P	137	VAL	2.3
1	P	218	VAL	2.3
1	P	155	THR	2.2
1	O	106	GLU	2.2
1	P	30	GLU	2.2
1	O	216	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	55	LYS	2.2
1	P	71	GLY	2.2
1	P	171	GLY	2.2
1	P	45	HIS	2.2
1	O	113	LYS	2.2
1	P	117	LYS	2.2
1	O	197	LEU	2.2
1	P	23	GLY	2.2
1	P	88	GLY	2.2
1	P	16	ILE	2.2
1	P	63	ASN	2.2
1	P	41	LYS	2.2
1	P	119	VAL	2.2
1	P	170	LEU	2.2
1	P	172	LEU	2.2
1	P	274	ILE	2.2
1	P	128	ASP	2.1
1	P	221	VAL	2.1
1	O	215	ALA	2.1
1	P	67	MET	2.1
1	P	134	VAL	2.1
1	P	285	VAL	2.1
1	P	303	VAL	2.1
1	O	38	GLY	2.1
1	P	91	LYS	2.1
1	P	115	GLY	2.1
1	P	132	THR	2.1
1	P	272	LYS	2.1
1	O	81	ASN	2.0
1	P	160	ALA	2.0
1	O	23	GLY	2.0
1	P	77	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSD	P	154[A]	8/9	0.89	0.13	20,21,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSD	P	154[B]	8/9	0.89	0.13	20,21,26,27	1
1	CSD	O	154[A]	8/9	0.92	0.12	18,21,26,26	1
1	CSD	O	154[B]	8/9	0.92	0.12	18,21,26,26	1

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	O	341	5/5	0.83	0.18	31,32,35,35	5
3	K	O	343	1/1	0.88	0.14	37,37,37,37	0
4	PG4	P	344	13/13	0.88	0.14	40,45,52,54	0
2	SO4	O	342	5/5	0.90	0.16	27,27,29,29	5
2	SO4	P	341	5/5	0.90	0.12	32,33,35,36	5
3	K	P	343	1/1	0.93	0.12	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.