



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:23 AM GMT

PDB ID : 1CF2  
Title : THREE-DIMENSIONAL STRUCTURE OF D-GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE FROM THE HYPERTHERMOPHILIC ARCHAEON METHANOTHERMUS FERVIDUS  
Authors : Charron, C.; Talfournier, F.; Isupov, M.N.; Branlant, G.; Littlechild, J.A.; Vitoux, B.; Aubry, A.  
Deposited on : 1999-03-24  
Resolution : 2.10 Å(reported)

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

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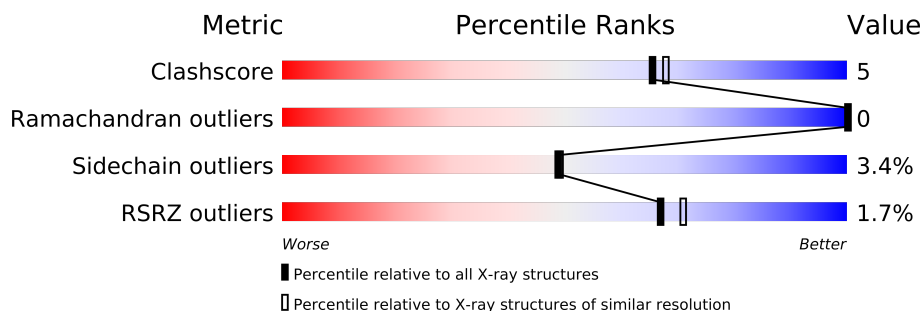
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	337	
1	P	337	
1	Q	337	
1	R	337	

## 2 Entry composition i

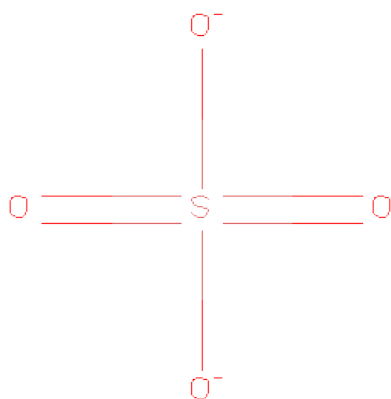
There are 4 unique types of molecules in this entry. The entry contains 11620 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			
1	R	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			
1	O	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			
1	Q	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



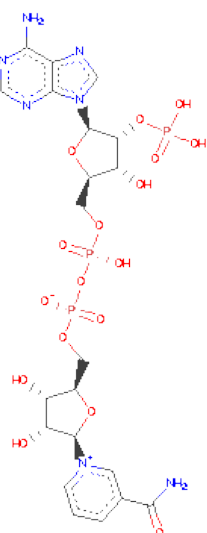
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	R	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	Q	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	217	Total	O	0	0
			217	217		
4	P	259	Total	O	0	0
			259	259		
4	Q	250	Total	O	0	0
			250	250		

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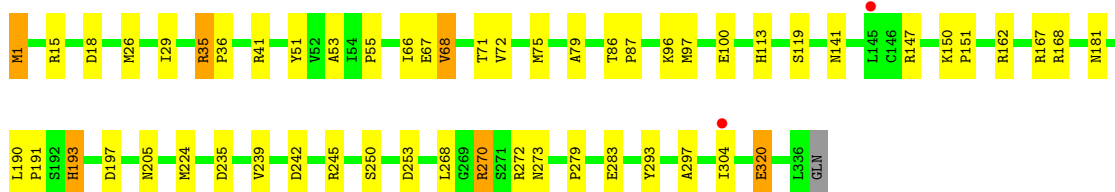
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	234	Total 234	O 234	0	0

### 3 Residue-property plots

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

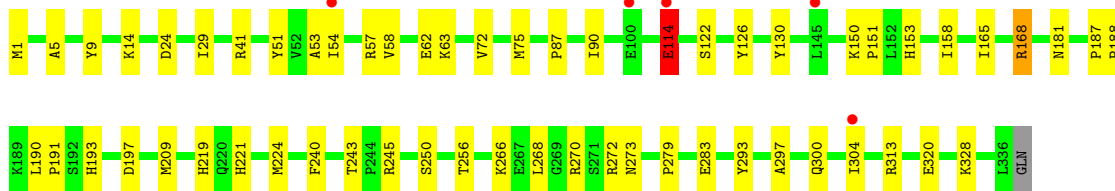
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE)

Chain P: 



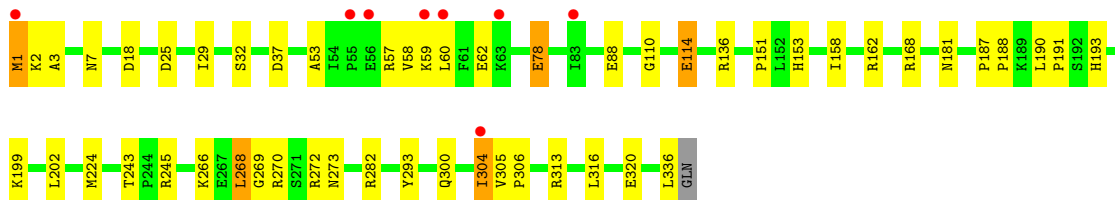
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE)

Chain R: 



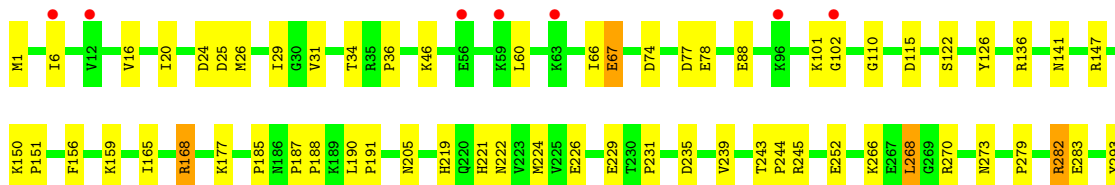
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE)

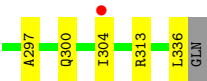
Chain O: 



- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE)

Chain Q: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.66Å 153.28Å 74.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 33.10 – 2.01	Depositor EDS
% Data completeness (in resolution range)	91.7 (10.00-2.10) 85.6 (33.10-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	5.60	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.257 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 89935 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.57% 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: NAP, 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	0.47	0/2654	1.19	12/3593 (0.3%)
1	P	0.51	0/2654	1.21	11/3593 (0.3%)
1	Q	0.48	0/2654	1.20	14/3593 (0.4%)
1	R	0.51	0/2654	1.18	6/3593 (0.2%)
All	All	0.49	0/10616	1.20	43/14372 (0.3%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	245	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	O	272	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	P	15	ARG	NE-CZ-NH1	-9.03	115.78	120.30
1	Q	245	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	R	245	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	Q	115	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	O	18	ASP	CB-CG-OD1	7.99	125.49	118.30
1	R	41	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	P	242	ASP	CB-CG-OD1	7.20	124.78	118.30
1	Q	147	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	P	147	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	O	282	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	P	245	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	Q	147	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	Q	168	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	Q	25	ASP	CB-CG-OD1	6.33	124.00	118.30
1	Q	24	ASP	CB-CG-OD1	6.22	123.90	118.30
1	R	313	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	R	272	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	O	1	MET	N-CA-CB	6.11	121.59	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	18	ASP	CB-CG-OD1	5.97	123.68	118.30
1	R	114	GLU	CA-CB-CG	5.96	126.51	113.40
1	P	270	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	O	313	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	P	253	ASP	CB-CG-OD1	5.79	123.51	118.30
1	Q	26	MET	CA-CB-CG	5.77	123.11	113.30
1	P	162	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	P	41	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	P	68	VAL	CA-CB-CG1	5.46	119.09	110.90
1	P	167	ARG	CD-NE-CZ	5.46	131.24	123.60
1	O	245	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	Q	168	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	Q	136	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	Q	282	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	O	78	GLU	CB-CA-C	-5.16	100.08	110.40
1	Q	34	THR	N-CA-CB	5.15	120.08	110.30
1	O	136	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	Q	313	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	O	162	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	O	282	ARG	CD-NE-CZ	5.07	130.70	123.60
1	O	25	ASP	CB-CG-OD1	5.06	122.86	118.30
1	O	37	ASP	CB-CG-OD1	5.04	122.83	118.30
1	Q	74	ASP	CB-CG-OD1	-5.00	113.80	118.30

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	2612	0	2637	28	0
1	P	2612	0	2637	25	0
1	Q	2612	0	2637	31	1
1	R	2612	0	2637	29	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	5	0	0	1	0
2	R	5	0	0	0	0
3	O	48	0	25	1	0
3	P	48	0	25	3	0
3	Q	48	0	25	1	0
3	R	48	0	25	1	0
4	O	217	0	0	7	0
4	P	259	0	0	2	0
4	Q	250	0	0	1	0
4	R	234	0	0	1	0
All	All	11620	0	10648	110	1

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 5.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:153:HIS:HD2	1:O:158:ILE:H	1.08	1.00
1:Q:159:LYS:HD3	1:Q:226:GLU:HB3	1.62	0.80
1:O:273:ASN:ND2	1:Q:273:ASN:ND2	2.34	0.76
1:O:153:HIS:CD2	1:O:158:ILE:H	2.00	0.75
1:R:250:SER:HB2	1:R:283:GLU:OE2	1.90	0.71
1:O:88:GLU:HG2	1:O:110:GLY:HA3	1.70	0.71
1:Q:266:LYS:HG2	1:Q:273:ASN:ND2	2.09	0.68
1:O:57:ARG:HD3	4:O:1191:HOH:O	1.95	0.67
1:P:320:GLU:HG3	4:P:1157:HOH:O	1.96	0.65
1:R:114:GLU:HG3	4:R:1117:HOH:O	1.98	0.63
1:R:150:LYS:HB3	1:R:151:PRO:HD3	1.80	0.63
1:R:266:LYS:HG2	1:R:273:ASN:ND2	2.15	0.62
1:R:266:LYS:HG2	1:R:273:ASN:HD22	1.64	0.60
1:O:114:GLU:H	1:O:114:GLU:CD	2.03	0.60
1:O:190:LEU:HB3	1:O:191:PRO:HA	1.82	0.60
1:O:58:VAL:O	1:O:62:GLU:HG3	2.04	0.57
1:O:268:LEU:HD21	1:O:336:LEU:HD11	1.85	0.57
1:R:190:LEU:HB3	1:R:191:PRO:HA	1.86	0.57
1:O:3:ALA:HB1	1:O:29:ILE:HG12	1.86	0.57
1:O:266:LYS:HG2	1:O:273:ASN:ND2	2.20	0.57
1:O:53:ALA:HB3	4:O:1191:HOH:O	2.06	0.56
1:Q:159:LYS:HD3	1:Q:226:GLU:CB	2.33	0.56
1:O:59:LYS:HA	1:O:62:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:273:ASN:ND2	1:R:273:ASN:ND2	2.54	0.55
1:R:279:PRO:HD2	1:R:297:ALA:O	2.07	0.55
1:O:187:PRO:HB2	1:O:188:PRO:HD2	1.89	0.55
1:Q:224:MET:HG2	1:Q:293:TYR:CD1	2.43	0.54
1:R:224:MET:HG2	1:R:293:TYR:CD1	2.44	0.53
1:P:35:ARG:HG2	3:P:340:NAP:O2X	2.09	0.53
1:P:96:LYS:O	1:P:100:GLU:HG3	2.08	0.53
1:P:193:HIS:HB3	4:P:1040:HOH:O	2.09	0.52
1:P:113:HIS:HD2	1:P:119:SER:OG	1.91	0.52
1:P:235:ASP:O	1:P:239:VAL:HG23	2.10	0.52
1:P:190:LEU:HB3	1:P:191:PRO:HA	1.92	0.52
1:P:55:PRO:HB3	1:P:71:THR:HG21	1.91	0.52
1:Q:190:LEU:HB3	1:Q:191:PRO:HA	1.90	0.51
1:Q:16:VAL:O	1:Q:20:ILE:HG12	2.12	0.50
1:R:58:VAL:O	1:R:62:GLU:HG3	2.12	0.50
4:O:1150:HOH:O	1:Q:46:LYS:HE3	2.12	0.50
1:Q:268:LEU:HD21	1:Q:336:LEU:HD11	1.94	0.50
1:Q:141:ASN:HB2	2:Q:1004:SO4:O2	2.12	0.50
1:R:24:ASP:OD1	1:R:328:LYS:NZ	2.45	0.49
1:O:320:GLU:HG3	4:O:1025:HOH:O	2.13	0.49
1:R:54:ILE:HG13	1:R:57:ARG:HG3	1.95	0.49
1:R:122:SER:O	1:R:126:TYR:HB2	2.13	0.49
1:Q:235:ASP:O	1:Q:239:VAL:HG23	2.13	0.48
1:Q:279:PRO:HD2	1:Q:297:ALA:O	2.13	0.48
1:O:300:GLN:O	3:O:340:NAP:H4N	2.14	0.48
1:Q:29:ILE:HD13	1:Q:78:GLU:HB2	1.95	0.48
1:Q:88:GLU:HG2	1:Q:110:GLY:HA3	1.95	0.48
1:O:2:LYS:HD2	1:O:316:LEU:HD13	1.95	0.48
1:Q:300:GLN:O	3:Q:340:NAP:H4N	2.14	0.47
1:R:256:THR:O	1:Q:185:PRO:HD2	2.15	0.47
3:P:340:NAP:N7N	3:P:340:NAP:O1N	2.48	0.46
1:P:141:ASN:HB2	2:P:1001:SO4:O2	2.16	0.46
1:R:130:TYR:CZ	1:R:320:GLU:HG2	2.51	0.46
1:P:272:ARG:O	1:P:273:ASN:HB2	2.16	0.46
1:O:153:HIS:HE1	4:O:1187:HOH:O	1.99	0.46
1:Q:187:PRO:HB2	1:Q:188:PRO:HD2	1.98	0.45
1:Q:252:GLU:HG3	1:Q:283:GLU:OE2	2.16	0.45
1:R:51:TYR:CG	1:R:75:MET:HB2	2.51	0.45
1:P:67:GLU:H	1:P:67:GLU:CD	2.19	0.45
1:O:304:ILE:HD13	1:O:304:ILE:H	1.82	0.45
1:O:181:ASN:HB2	4:O:1216:HOH:O	2.16	0.45
1:P:36:PRO:HB2	1:P:66:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:150:LYS:N	1:P:151:PRO:HD2	2.33	0.44
1:O:305:VAL:HB	1:O:306:PRO:HD3	2.00	0.44
1:R:53:ALA:HA	1:R:72:VAL:HG23	1.99	0.44
1:O:153:HIS:HD2	1:O:158:ILE:N	1.93	0.44
1:Q:67:GLU:HG2	4:Q:1010:HOH:O	2.18	0.44
1:Q:266:LYS:HA	1:Q:273:ASN:HB3	2.00	0.44
1:P:279:PRO:HD2	1:P:297:ALA:O	2.18	0.43
1:Q:156:PHE:CE1	1:Q:231:PRO:HB3	2.53	0.43
1:Q:122:SER:O	1:Q:126:TYR:HB2	2.19	0.43
1:R:300:GLN:O	3:R:340:NAP:H4N	2.19	0.43
1:O:199:LYS:HA	1:O:202:LEU:O	2.19	0.43
1:P:86:THR:HB	1:P:87:PRO:HD2	2.01	0.43
1:Q:6:ILE:HB	1:Q:31:VAL:HG12	2.01	0.42
1:O:269:GLY:HA2	4:O:1134:HOH:O	2.19	0.42
1:Q:243:THR:HA	1:Q:244:PRO:HD3	1.96	0.42
1:P:86:THR:HB	1:P:87:PRO:CD	2.49	0.42
1:P:53:ALA:HA	1:P:72:VAL:HG23	2.00	0.42
1:R:165:ILE:HD12	1:R:221:HIS:CD2	2.54	0.42
1:O:224:MET:HG2	1:O:293:TYR:CD1	2.55	0.42
1:R:266:LYS:HA	1:R:273:ASN:HB3	2.01	0.42
1:O:304:ILE:H	1:O:304:ILE:CD1	2.33	0.42
1:R:168:ARG:HG3	1:R:219:HIS:CE1	2.54	0.41
1:O:7:ASN:HA	1:O:32:SER:OG	2.20	0.41
1:P:250:SER:HB2	1:P:283:GLU:OE2	2.19	0.41
1:P:29:ILE:HD11	1:P:79:ALA:HB2	2.02	0.41
1:Q:177:LYS:HE2	1:Q:177:LYS:HB3	1.83	0.41
1:Q:165:ILE:HD12	1:Q:221:HIS:CD2	2.55	0.41
1:P:1:MET:HG2	1:P:26:MET:N	2.35	0.41
1:P:224:MET:HG2	1:P:293:TYR:CD1	2.56	0.41
1:R:9:TYR:CE1	1:R:14:LYS:HA	2.55	0.41
1:Q:150:LYS:N	1:Q:151:PRO:HD2	2.35	0.41
3:P:340:NAP:H2N	3:P:340:NAP:H2D	1.77	0.41
1:R:153:HIS:HA	1:R:158:ILE:HG13	2.03	0.41
1:P:51:TYR:CE1	1:P:75:MET:HG3	2.56	0.41
1:R:209:MET:HE2	1:Q:222:ASN:HB3	2.02	0.41
1:R:87:PRO:O	1:R:90:ILE:HB	2.21	0.41
1:Q:219:HIS:CD2	1:Q:300:GLN:HB3	2.56	0.41
1:P:53:ALA:HA	1:P:72:VAL:CG2	2.50	0.41
1:R:240:PHE:HA	1:R:243:THR:HG22	2.02	0.40
1:P:181:ASN:ND2	1:R:181:ASN:HD22	2.18	0.40
1:O:151:PRO:HG3	1:O:243:THR:OG1	2.21	0.40
1:R:5:ALA:HB2	1:R:29:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:36:PRO:HB2	1:Q:66:ILE:HD12	2.03	0.40
1:Q:77:ASP:OD1	1:Q:101:LYS:NZ	2.41	0.40
1:R:187:PRO:HB2	1:R:188:PRO:HD2	2.03	0.40

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	Distance(Å)	Clash(Å)
1:R:63:LYS:NZ	1:Q:102:GLY:O[4_555]	2.18	0.02

## 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	334/337 (99%)	324 (97%)	10 (3%)	0	100	100
1	P	334/337 (99%)	324 (97%)	10 (3%)	0	100	100
1	Q	334/337 (99%)	326 (98%)	8 (2%)	0	100	100
1	R	334/337 (99%)	323 (97%)	11 (3%)	0	100	100
All	All	1336/1348 (99%)	1297 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	290/291 (100%)	281 (97%)	9 (3%)	52	54
1	P	290/291 (100%)	278 (96%)	12 (4%)	41	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	290/291 (100%)	280 (97%)	10 (3%)	49	49
1	R	290/291 (100%)	282 (97%)	8 (3%)	56	59
All	All	1160/1164 (100%)	1121 (97%)	39 (3%)	49	49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	1	MET
1	P	35	ARG
1	P	68	VAL
1	P	97	MET
1	P	168	ARG
1	P	193	HIS
1	P	197	ASP
1	P	205	ASN
1	P	268	LEU
1	P	270	ARG
1	P	304	ILE
1	P	320	GLU
1	R	1	MET
1	R	114	GLU
1	R	168	ARG
1	R	193	HIS
1	R	197	ASP
1	R	268	LEU
1	R	270	ARG
1	R	304	ILE
1	O	1	MET
1	O	60	LEU
1	O	78	GLU
1	O	114	GLU
1	O	168	ARG
1	O	193	HIS
1	O	268	LEU
1	O	270	ARG
1	O	304	ILE
1	Q	1	MET
1	Q	60	LEU
1	Q	67	GLU
1	Q	168	ARG
1	Q	205	ASN

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Mol	Chain	Res	Type
1	Q	229	GLU
1	Q	268	LEU
1	Q	270	ARG
1	Q	282	ARG
1	Q	304	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	113	HIS
1	P	205	ASN
1	P	273	ASN
1	P	334	ASN
1	R	273	ASN
1	O	153	HIS
1	O	273	ASN
1	Q	22	GLN
1	Q	205	ASN
1	Q	273	ASN
1	Q	334	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	1003	-	4,4,4	0.96	0	6,6,6	0.32	0
3	NAP	O	340	-	52,52,52	1.04	3 (5%)	80,80,80	1.65	15 (18%)
2	SO4	P	1001	-	4,4,4	0.96	0	6,6,6	0.22	0
3	NAP	P	340	-	52,52,52	1.00	3 (5%)	80,80,80	1.69	12 (15%)
2	SO4	Q	1004	-	4,4,4	0.99	0	6,6,6	0.28	0
3	NAP	Q	340	-	52,52,52	0.96	2 (3%)	80,80,80	1.86	16 (20%)
2	SO4	R	1002	-	4,4,4	0.97	0	6,6,6	0.18	0
3	NAP	R	340	-	52,52,52	0.92	2 (3%)	80,80,80	1.77	13 (16%)

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	1003	-	-	0/0/0/0	0/0/0/0
3	NAP	O	340	-	-	0/35/67/67	0/3/5/5
2	SO4	P	1001	-	-	0/0/0/0	0/0/0/0
3	NAP	P	340	-	-	0/35/67/67	0/3/5/5
2	SO4	Q	1004	-	-	0/0/0/0	0/0/0/0
3	NAP	Q	340	-	-	0/35/67/67	0/3/5/5
2	SO4	R	1002	-	-	0/0/0/0	0/0/0/0
3	NAP	R	340	-	-	0/35/67/67	0/3/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	340	NAP	C3N-C7N	3.90	1.57	1.50
3	R	340	NAP	C3N-C7N	3.62	1.56	1.50
3	Q	340	NAP	C3N-C7N	3.55	1.56	1.50
3	P	340	NAP	C3N-C7N	3.52	1.56	1.50
3	Q	340	NAP	C6N-N1N	2.77	1.43	1.35
3	R	340	NAP	C6N-N1N	2.72	1.43	1.35
3	O	340	NAP	C6N-N1N	2.66	1.43	1.35
3	P	340	NAP	C6N-N1N	2.57	1.42	1.35
3	P	340	NAP	C2A-N1A	2.27	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	340	NAP	C2A-N1A	2.22	1.38	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	340	NAP	O7N-C7N-C3N	7.14	127.63	119.58
3	R	340	NAP	O4D-C1D-N1N	-5.95	101.86	107.95
3	O	340	NAP	C5N-C4N-C3N	-5.80	112.79	120.32
3	P	340	NAP	C5N-C4N-C3N	-5.72	112.89	120.32
3	P	340	NAP	C6N-C5N-C4N	5.57	128.30	119.44
3	Q	340	NAP	C5N-C4N-C3N	-5.49	113.19	120.32
3	R	340	NAP	C6N-C5N-C4N	5.48	128.14	119.44
3	Q	340	NAP	C6N-C5N-C4N	5.46	128.12	119.44
3	R	340	NAP	C5N-C4N-C3N	-5.42	113.29	120.32
3	O	340	NAP	C2N-C3N-C4N	5.35	124.37	118.31
3	R	340	NAP	C5N-C6N-N1N	-4.40	113.02	120.43
3	O	340	NAP	C6N-C5N-C4N	4.38	126.39	119.44
3	P	340	NAP	C5N-C6N-N1N	-4.29	113.20	120.43
3	Q	340	NAP	C5N-C6N-N1N	-4.18	113.39	120.43
3	R	340	NAP	C2N-C3N-C4N	4.14	123.00	118.31
3	R	340	NAP	O4D-C1D-C2D	-4.01	100.63	106.77
3	P	340	NAP	C2N-C3N-C4N	3.93	122.76	118.31
3	O	340	NAP	O7N-C7N-C3N	3.91	123.98	119.58
3	P	340	NAP	C1B-N9A-C4A	-3.62	120.38	126.64
3	O	340	NAP	O4B-C1B-N9A	-3.51	105.18	108.44
3	Q	340	NAP	C2N-C3N-C4N	3.45	122.22	118.31
3	Q	340	NAP	C3N-C7N-N7N	-3.38	113.92	117.77
3	Q	340	NAP	C1B-N9A-C4A	-3.36	120.82	126.64
3	Q	340	NAP	O4B-C1B-N9A	-3.35	105.33	108.44
3	Q	340	NAP	P2B-O2B-C2B	-3.23	115.16	121.96
3	P	340	NAP	C4A-C5A-N7A	3.19	112.26	109.52
3	Q	340	NAP	C8A-N9A-C1B	3.19	132.67	126.38
3	P	340	NAP	O4D-C1D-C2D	-3.07	102.06	106.77
3	R	340	NAP	C4N-C3N-C7N	-3.06	112.97	121.10
3	R	340	NAP	O4B-C1B-N9A	-3.05	105.60	108.44
3	Q	340	NAP	O4D-C1D-N1N	-3.04	104.84	107.95
3	O	340	NAP	C2D-C1D-N1N	3.03	118.98	113.86
3	P	340	NAP	P2B-O2B-C2B	-3.00	115.64	121.96
3	O	340	NAP	C4N-C3N-C7N	-2.98	113.19	121.10
3	P	340	NAP	C4N-C3N-C7N	-2.90	113.38	121.10
3	Q	340	NAP	O7N-C7N-N7N	-2.87	118.44	122.59
3	R	340	NAP	P2B-O2B-C2B	-2.84	115.99	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	340	NAP	C5N-C6N-N1N	-2.79	115.72	120.43
3	O	340	NAP	O2N-PN-O1N	-2.67	110.67	118.72
3	R	340	NAP	C1B-N9A-C4A	-2.66	122.03	126.64
3	O	340	NAP	C1B-N9A-C4A	-2.63	122.08	126.64
3	Q	340	NAP	C4N-C3N-C7N	-2.62	114.13	121.10
3	P	340	NAP	C8A-N9A-C1B	2.61	131.53	126.38
3	O	340	NAP	C4A-C5A-N7A	2.55	111.70	109.52
3	Q	340	NAP	C2D-C1D-N1N	2.49	118.07	113.86
3	O	340	NAP	C8A-N9A-C1B	2.42	131.16	126.38
3	O	340	NAP	P2B-O2B-C2B	-2.34	117.03	121.96
3	O	340	NAP	C3N-C7N-N7N	-2.29	115.17	117.77
3	P	340	NAP	O2N-PN-O5D	2.28	117.60	108.19
3	Q	340	NAP	O3X-P2B-O2B	2.20	113.42	107.09
3	P	340	NAP	O4B-C1B-N9A	-2.18	106.42	108.44
3	Q	340	NAP	O2N-PN-O1N	-2.17	112.18	118.72
3	R	340	NAP	O2N-PN-O1N	-2.14	112.25	118.72
3	R	340	NAP	C2D-C3D-C4D	-2.13	98.40	102.65
3	O	340	NAP	O3X-P2B-O2B	2.02	112.90	107.09
3	R	340	NAP	C8A-N9A-C1B	2.01	130.35	126.38

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	336/337 (99%)	-0.02	8 (2%)	56	61	22, 37, 60, 86	0
1	P	336/337 (99%)	-0.11	2 (0%)	86	90	22, 33, 53, 70	0
1	Q	336/337 (99%)	-0.07	8 (2%)	56	61	21, 36, 54, 81	0
1	R	336/337 (99%)	-0.08	5 (1%)	70	74	20, 36, 54, 75	0
All	All	1344/1348 (99%)	-0.07	23 (1%)	67	71	20, 35, 55, 86	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	3.3
1	Q	63	LYS	3.1
1	P	304	ILE	2.9
1	Q	56	GLU	2.7
1	O	56	GLU	2.7
1	R	304	ILE	2.7
1	P	145	LEU	2.5
1	O	55	PRO	2.3
1	Q	12	VAL	2.2
1	O	60	LEU	2.2
1	Q	304	ILE	2.1
1	R	100	GLU	2.1
1	R	145	LEU	2.1
1	O	63	LYS	2.1
1	O	304	ILE	2.1
1	Q	6	ILE	2.1
1	O	59	LYS	2.1
1	R	114	GLU	2.0
1	O	83	ILE	2.0
1	Q	102	GLY	2.0
1	Q	59	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	96	LYS	2.0
1	R	54	ILE	2.0

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	Q	1004	5/5	0.13	0.53	61,62,64,65	0
2	SO4	R	1002	5/5	0.13	-0.57	55,56,58,59	0
3	NAP	R	340	48/48	0.09	-0.73	22,39,48,55	0
3	NAP	P	340	48/48	0.09	-0.74	23,33,40,41	0
3	NAP	Q	340	48/48	0.08	-0.82	22,34,43,48	0
3	NAP	O	340	48/48	0.10	-0.82	24,37,45,47	0
2	SO4	O	1003	5/5	0.09	-1.32	46,49,51,52	0
2	SO4	P	1001	5/5	0.09	-2.82	69,69,71,74	0

## 6.5 Other polymers

There are no such residues in this entry.