



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:14 AM GMT

PDB ID : 2G82
Title : High Resolution Structures of *Thermus aquaticus* Glyceraldehyde-3-Phosphate Dehydrogenase: Role of 220's Loop Motion in Catalysis
Authors : Jenkins, J.L.; Buencamino, R.; Tanner, J.J.
Deposited on : 2006-03-01
Resolution : 1.65 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

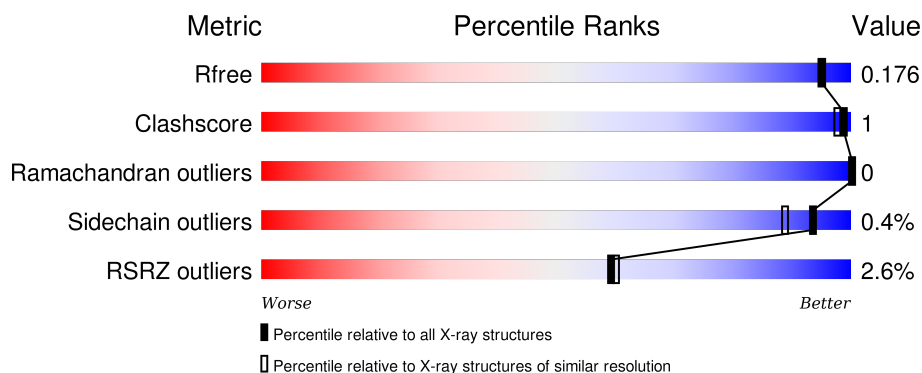
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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.



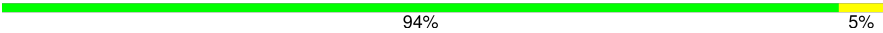
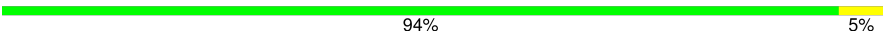

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	331	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	B	331	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
1	C	331	<div> <div>96%</div> <div>.</div> </div>
1	D	331	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
1	O	331	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	331	 94% 5%
1	Q	331	 94% 5%
1	R	331	 2% 96% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	A	336	-	-	-	X
3	NAD	B	336	-	-	-	X
3	NAD	D	336	-	-	-	X
4	PGE	C	1700	-	-	-	X
5	IPA	C	1800	-	-	-	X
5	IPA	Q	1801	-	-	-	X
6	GOL	D	3504	-	-	-	X
6	GOL	Q	3503	-	-	-	X
6	GOL	R	3502	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22023 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	330	Total	C	N	O	S	0	4	0
			2499	1582	436	474	7			
1	P	330	Total	C	N	O	S	0	4	0
			2522	1594	443	478	7			
1	Q	330	Total	C	N	O	S	0	4	0
			2515	1591	441	476	7			
1	R	330	Total	C	N	O	S	0	4	0
			2514	1591	440	476	7			
1	A	330	Total	C	N	O	S	0	4	0
			2492	1577	436	472	7			
1	B	330	Total	C	N	O	S	0	4	0
			2505	1586	436	476	7			
1	C	330	Total	C	N	O	S	0	4	0
			2511	1591	439	474	7			
1	D	330	Total	C	N	O	S	0	4	0
			2490	1579	437	467	7			

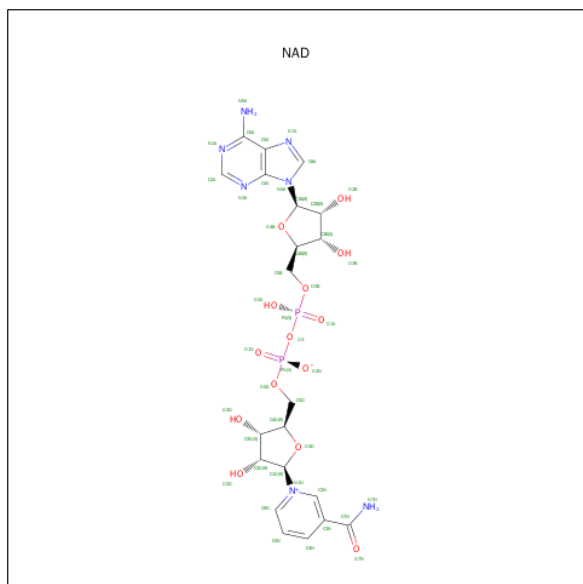
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
P	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
Q	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
R	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
A	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
B	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
C	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361
D	149	CSD	CYS	MODIFIED RESIDUE	UNP P00361

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



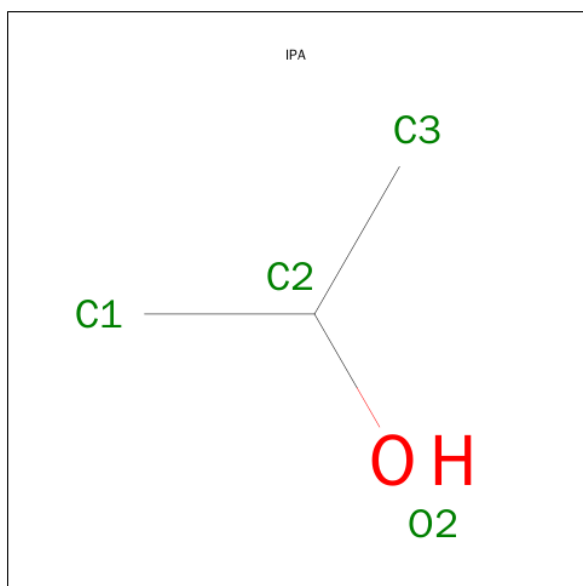
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	3	1		
5	Q	1	Total	C	O	0	0
			4	3	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	R	1	Total	C	O	0	0
			6	3	3		
6	Q	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

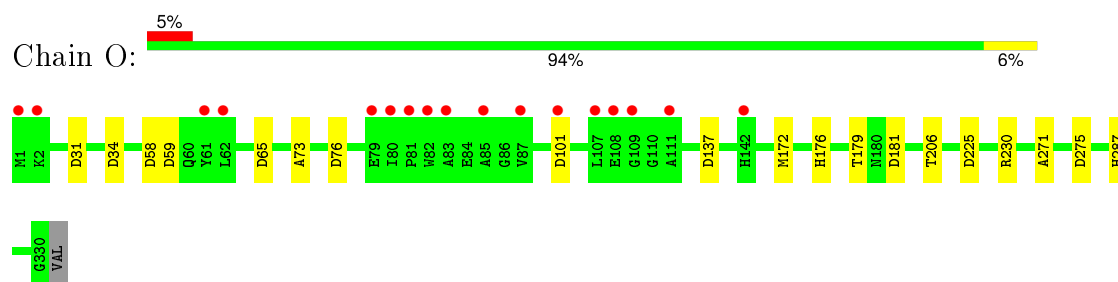
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	175	Total	O	0	0
			175	175		
7	B	145	Total	O	0	0
			145	145		
7	C	226	Total	O	0	0
			226	226		
7	D	147	Total	O	0	0
			147	147		
7	O	189	Total	O	0	0
			189	189		
7	P	236	Total	O	0	0
			236	236		
7	Q	240	Total	O	0	0
			240	240		
7	R	228	Total	O	0	0
			228	228		

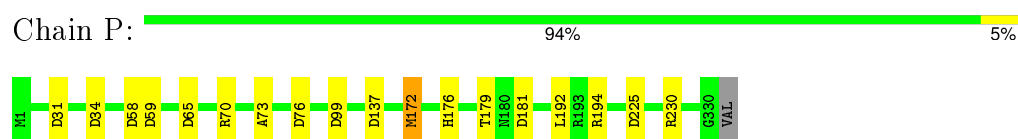
3 Residue-property plots

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.

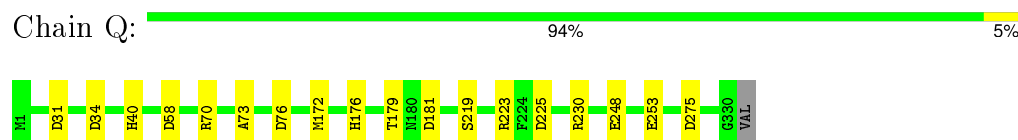
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



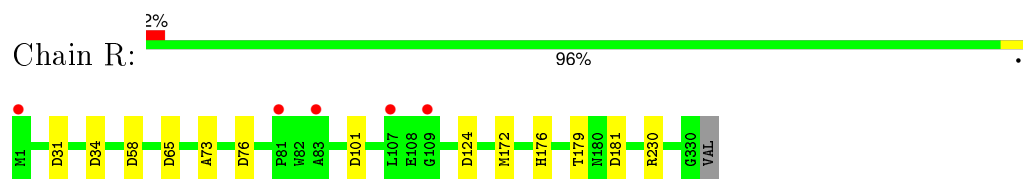
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



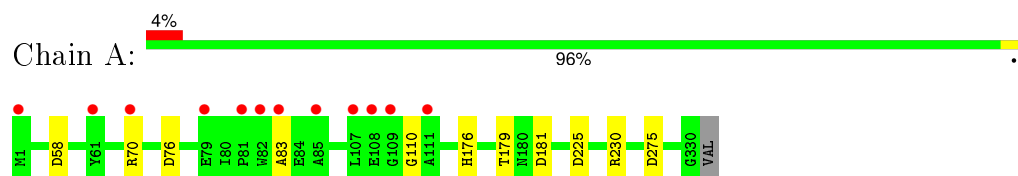
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



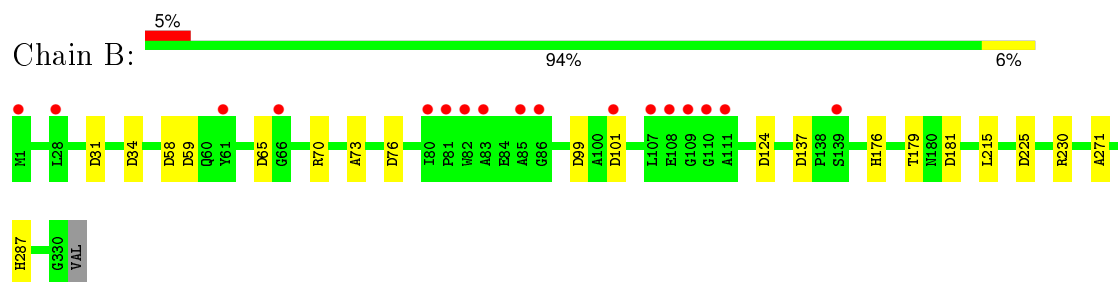
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



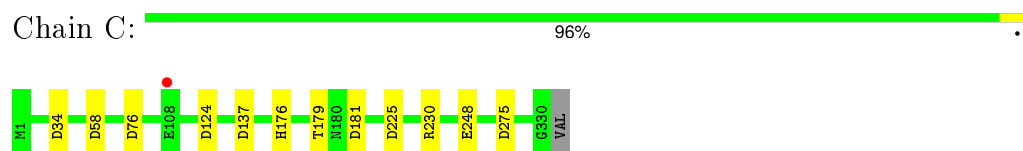
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



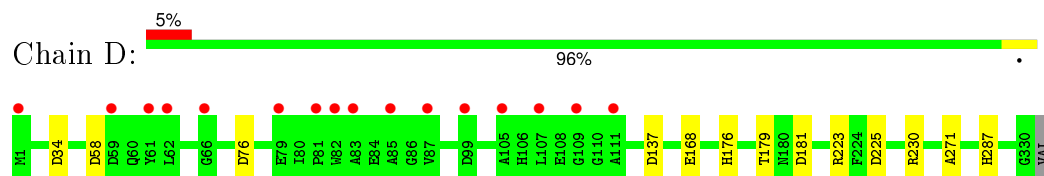
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.55Å 147.40Å 147.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.94 – 1.65 66.02 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.94-1.65) 98.2 (66.02-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.158 , 0.172 0.165 , 0.176	Depositor DCC
R_{free} test set	18298 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
Estimated twinning fraction	0.006 for -h,l,k 0.003 for -l,-k,-h 0.004 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 364003 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22023	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, PGE, NAD, CSD, IPA, NA

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	A	0.37	0/2450	0.71	4/3336 (0.1%)
1	B	0.37	0/2463	0.73	10/3351 (0.3%)
1	C	0.38	0/2469	0.72	7/3357 (0.2%)
1	D	0.38	0/2448	0.71	5/3332 (0.2%)
1	O	0.39	1/2457 (0.0%)	0.73	9/3344 (0.3%)
1	P	0.42	1/2480 (0.0%)	0.74	8/3371 (0.2%)
1	Q	0.42	1/2473 (0.0%)	0.72	5/3362 (0.1%)
1	R	0.41	1/2472 (0.0%)	0.73	6/3361 (0.2%)
All	All	0.39	4/19712 (0.0%)	0.72	54/26814 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	172	MET	SD-CE	-8.39	1.30	1.77
1	P	172	MET	SD-CE	-8.18	1.32	1.77
1	Q	172	MET	SD-CE	-6.99	1.38	1.77
1	O	172	MET	SD-CE	-5.96	1.44	1.77

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ASP	CB-CG-OD2	6.99	124.59	118.30
1	R	58	ASP	CB-CG-OD2	6.63	124.27	118.30
1	R	101	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	58	ASP	CB-CG-OD2	6.46	124.12	118.30
1	P	99	ASP	CB-CG-OD2	6.41	124.06	118.30
1	P	59	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	34	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	59	ASP	CB-CG-OD2	6.33	124.00	118.30
1	O	137	ASP	CB-CG-OD2	6.30	123.97	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ASP	CB-CG-OD2	6.29	123.97	118.30
1	C	225	ASP	CB-CG-OD2	6.25	123.92	118.30
1	O	275	ASP	CB-CG-OD2	6.24	123.92	118.30
1	P	137	ASP	CB-CG-OD2	6.22	123.90	118.30
1	Q	275	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	76	ASP	CB-CG-OD2	6.16	123.85	118.30
1	O	58	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	76	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	275	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	225	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	225	ASP	CB-CG-OD2	5.94	123.64	118.30
1	D	137	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	58	ASP	CB-CG-OD2	5.85	123.57	118.30
1	P	58	ASP	CB-CG-OD2	5.84	123.55	118.30
1	Q	76	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	34	ASP	CB-CG-OD2	5.82	123.53	118.30
1	O	65	ASP	CB-CG-OD2	5.81	123.53	118.30
1	O	76	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	275	ASP	CB-CG-OD2	5.76	123.49	118.30
1	R	65	ASP	CB-CG-OD2	5.68	123.42	118.30
1	C	124	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	225	ASP	CB-CG-OD2	5.65	123.39	118.30
1	D	76	ASP	CB-CG-OD2	5.65	123.39	118.30
1	O	101	ASP	CB-CG-OD2	5.63	123.36	118.30
1	P	34	ASP	CB-CG-OD2	5.60	123.34	118.30
1	R	34	ASP	CB-CG-OD2	5.57	123.31	118.30
1	R	76	ASP	CB-CG-OD2	5.56	123.31	118.30
1	Q	225	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	58	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	137	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	65	ASP	CB-CG-OD2	5.41	123.17	118.30
1	O	225	ASP	CB-CG-OD2	5.38	123.14	118.30
1	Q	34	ASP	CB-CG-OD2	5.38	123.14	118.30
1	P	65	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	101	ASP	CB-CG-OD2	5.34	123.11	118.30
1	P	225	ASP	CB-CG-OD2	5.33	123.10	118.30
1	R	124	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	124	ASP	CB-CG-OD2	5.26	123.04	118.30
1	O	34	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	137	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	76	ASP	CB-CG-OD2	5.19	122.97	118.30
1	P	76	ASP	CB-CG-OD2	5.19	122.97	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	58	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	34	ASP	CB-CG-OD2	5.14	122.93	118.30
1	O	59	ASP	CB-CG-OD2	5.10	122.89	118.30

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	A	2492	0	2471	3	0
1	B	2505	0	2489	4	0
1	C	2511	0	2504	2	0
1	D	2490	0	2473	5	0
1	O	2499	0	2481	5	0
1	P	2522	0	2520	7	0
1	Q	2515	0	2514	6	0
1	R	2514	0	2509	3	0
2	C	1	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
3	O	44	0	26	0	0
3	P	44	0	26	0	0
3	Q	44	0	26	0	0
3	R	44	0	26	0	0
4	C	10	0	14	0	0
5	C	4	0	8	0	0
5	Q	4	0	8	0	0
6	D	6	0	8	0	0
6	Q	6	0	8	0	0
6	R	6	0	8	0	0
7	A	175	0	0	0	0
7	B	145	0	0	0	0
7	C	226	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	147	0	0	0	0
7	O	189	0	0	1	0
7	P	236	0	0	0	0
7	Q	240	0	0	0	0
7	R	228	0	0	0	0
All	All	22023	0	20223	33	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 1.

All (33) 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:179:THR:OG1	1:O:181[C]:ASP:OD1	2.01	0.78
1:D:179:THR:OG1	1:D:181[C]:ASP:OD2	2.01	0.77
1:P:181[C]:ASP:OD1	1:P:194[C]:ARG:NH1	2.19	0.76
1:C:179:THR:OG1	1:C:181[C]:ASP:OD2	2.09	0.71
1:R:179:THR:OG1	1:R:181[C]:ASP:OD2	2.13	0.67
1:Q:179:THR:OG1	1:Q:181[C]:ASP:OD2	2.15	0.63
1:A:179:THR:OG1	1:A:181[C]:ASP:OD1	2.24	0.55
1:P:179:THR:OG1	1:P:181[C]:ASP:OD2	2.26	0.54
1:Q:253:GLU:OE1	1:D:223:ARG:NE	2.38	0.54
1:D:176:HIS:HB3	1:D:230[B]:ARG:HD3	1.90	0.53
1:O:176:HIS:HB3	1:O:230[B]:ARG:HD3	1.91	0.52
1:R:176:HIS:HB3	1:R:230[B]:ARG:HD3	1.92	0.51
1:B:271:ALA:HB2	1:B:287:HIS:CD2	2.49	0.48
1:P:192:LEU:HB3	1:Q:40:HIS:CD2	2.50	0.47
1:A:176:HIS:HB3	1:A:230[B]:ARG:HD3	1.97	0.46
1:Q:176:HIS:HB3	1:Q:230[B]:ARG:HD3	1.96	0.46
1:C:176:HIS:HB3	1:C:230[B]:ARG:HD3	1.97	0.46
1:O:271:ALA:HB2	1:O:287:HIS:CD2	2.51	0.45
1:D:271:ALA:HB2	1:D:287:HIS:CD2	2.52	0.45
1:B:176:HIS:HB3	1:B:230[B]:ARG:HD3	1.99	0.45
1:A:83:ALA:HB2	1:A:110:GLY:HA3	1.99	0.44
1:O:206[C]:THR:HG22	7:O:441:HOH:O	2.17	0.44
1:Q:219:SER:O	1:Q:223:ARG:HD3	2.16	0.44
1:P:172:MET:HE2	1:P:172:MET:HB2	1.91	0.44
1:B:31:ASP:O	1:B:73:ALA:HA	2.18	0.43
1:P:31:ASP:O	1:P:73:ALA:HA	2.19	0.43
1:B:179:THR:OG1	1:B:181[C]:ASP:OD2	2.36	0.43
1:O:31:ASP:O	1:O:73:ALA:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:31:ASP:O	1:R:73:ALA:HA	2.20	0.41
1:Q:31:ASP:O	1:Q:73:ALA:HA	2.20	0.41
1:P:176:HIS:HB3	1:P:230[B]:ARG:HD3	2.04	0.40
1:P:181[C]:ASP:CG	1:P:194[C]:ARG:NH1	2.74	0.40
1:D:168:GLU:O	1:D:223:ARG:HD3	2.22	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	A	331/331 (100%)	323 (98%)	8 (2%)	0	100	100
1	B	331/331 (100%)	318 (96%)	13 (4%)	0	100	100
1	C	331/331 (100%)	321 (97%)	10 (3%)	0	100	100
1	D	331/331 (100%)	320 (97%)	11 (3%)	0	100	100
1	O	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	P	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	Q	331/331 (100%)	320 (97%)	11 (3%)	0	100	100
1	R	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
All	All	2648/2648 (100%)	2568 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	A	243/264 (92%)	242 (100%)	1 (0%)	93	89
1	B	245/264 (93%)	243 (99%)	2 (1%)	86	76
1	C	245/264 (93%)	244 (100%)	1 (0%)	93	89
1	D	240/264 (91%)	240 (100%)	0	100	100
1	O	244/264 (92%)	244 (100%)	0	100	100
1	P	249/264 (94%)	248 (100%)	1 (0%)	93	89
1	Q	248/264 (94%)	246 (99%)	2 (1%)	86	76
1	R	247/264 (94%)	247 (100%)	0	100	100
All	All	1961/2112 (93%)	1954 (100%)	7 (0%)	93	89

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

Mol	Chain	Res	Type
1	P	70	ARG
1	Q	70	ARG
1	Q	248	GLU
1	A	70	ARG
1	B	70	ARG
1	B	215	LEU
1	C	248	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	255	ASN
1	P	255	ASN
1	Q	255	ASN
1	R	255	ASN
1	A	255	ASN
1	B	255	ASN
1	C	255	ASN
1	D	255	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	A	149	1	3,7,8	1.13	0	3,8,10	2.04	1 (33%)
1	CSD	B	149	1	3,7,8	1.05	0	3,8,10	1.96	1 (33%)
1	CSD	C	149	1	3,7,8	1.02	0	3,8,10	1.85	1 (33%)
1	CSD	D	149	1	3,7,8	1.03	0	3,8,10	1.81	1 (33%)
1	CSD	O	149	1	3,7,8	1.13	0	3,8,10	2.26	2 (66%)
1	CSD	P	149	1	3,7,8	1.04	0	3,8,10	1.68	0
1	CSD	Q	149	1	3,7,8	1.04	0	3,8,10	1.74	0
1	CSD	R	149	1	3,7,8	1.01	0	3,8,10	1.28	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	A	149	1	-	0/2/6/8	0/0/0/0
1	CSD	B	149	1	-	0/2/6/8	0/0/0/0
1	CSD	C	149	1	-	0/2/6/8	0/0/0/0
1	CSD	D	149	1	-	0/2/6/8	0/0/0/0
1	CSD	O	149	1	-	0/2/6/8	0/0/0/0
1	CSD	P	149	1	-	0/2/6/8	0/0/0/0
1	CSD	Q	149	1	-	0/2/6/8	0/0/0/0
1	CSD	R	149	1	-	0/2/6/8	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	CSD	O-C-CA	-2.07	120.10	125.49
1	O	149	CSD	O-C-CA	-2.03	120.20	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	CSD	OD1-SG-CB	2.47	109.52	105.40
1	B	149	CSD	OD1-SG-CB	2.50	109.58	105.40
1	A	149	CSD	OD1-SG-CB	2.64	109.81	105.40
1	O	149	CSD	OD1-SG-CB	3.30	110.91	105.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
3	NAD	A	336	-	38,48,48	0.79	1 (2%)	47,73,73	1.78	6 (12%)
3	NAD	B	336	-	38,48,48	0.75	0	47,73,73	1.82	6 (12%)
4	PGE	C	1700	2	9,9,9	0.70	0	8,8,8	0.55	0
5	IPA	C	1800	-	3,3,3	0.60	0	3,3,3	0.15	0
3	NAD	C	336	-	38,48,48	0.92	1 (2%)	47,73,73	1.86	4 (8%)
3	NAD	D	336	-	38,48,48	0.93	2 (5%)	47,73,73	1.65	3 (6%)
6	GOL	D	3504	-	5,5,5	0.32	0	5,5,5	0.37	0
3	NAD	O	336	-	38,48,48	0.92	1 (2%)	47,73,73	1.74	5 (10%)
3	NAD	P	336	-	38,48,48	0.76	0	47,73,73	1.88	7 (14%)
5	IPA	Q	1801	-	3,3,3	0.58	0	3,3,3	0.13	0
3	NAD	Q	336	-	38,48,48	0.88	3 (7%)	47,73,73	1.74	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	Q	3503	-	5,5,5	0.33	0	5,5,5	0.51	0
3	NAD	R	336	-	38,48,48	0.80	1 (2%)	47,73,73	1.75	4 (8%)
6	GOL	R	3502	-	5,5,5	0.38	0	5,5,5	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	336	-	-	0/22/62/62	0/5/5/5
3	NAD	B	336	-	-	0/22/62/62	0/5/5/5
4	PGE	C	1700	2	-	0/7/7/7	0/0/0/0
5	IPA	C	1800	-	-	0/0/0/0	0/0/0/0
3	NAD	C	336	-	-	0/22/62/62	0/5/5/5
3	NAD	D	336	-	-	0/22/62/62	0/5/5/5
6	GOL	D	3504	-	-	0/4/4/4	0/0/0/0
3	NAD	O	336	-	-	0/22/62/62	0/5/5/5
3	NAD	P	336	-	-	0/22/62/62	0/5/5/5
5	IPA	Q	1801	-	-	0/0/0/0	0/0/0/0
3	NAD	Q	336	-	-	0/22/62/62	0/5/5/5
6	GOL	Q	3503	-	-	0/4/4/4	0/0/0/0
3	NAD	R	336	-	-	0/22/62/62	0/5/5/5
6	GOL	R	3502	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	336	NAD	C6N-N1N	2.04	1.40	1.35
3	D	336	NAD	O4B-C1B	2.15	1.43	1.41
3	R	336	NAD	O4D-C1D	2.16	1.43	1.41
3	Q	336	NAD	O4B-C1B	2.18	1.44	1.41
3	Q	336	NAD	O4D-C1D	2.20	1.44	1.41
3	D	336	NAD	O4D-C1D	2.26	1.44	1.41
3	A	336	NAD	O4D-C1D	2.47	1.44	1.41
3	O	336	NAD	O4D-C1D	3.17	1.45	1.41
3	C	336	NAD	O4D-C1D	3.25	1.45	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	336	NAD	N3A-C2A-N1A	-9.84	121.36	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	336	NAD	N3A-C2A-N1A	-9.79	121.40	128.89
3	R	336	NAD	N3A-C2A-N1A	-9.54	121.59	128.89
3	B	336	NAD	N3A-C2A-N1A	-9.50	121.62	128.89
3	O	336	NAD	N3A-C2A-N1A	-9.22	121.83	128.89
3	Q	336	NAD	N3A-C2A-N1A	-9.20	121.85	128.89
3	A	336	NAD	N3A-C2A-N1A	-9.10	121.93	128.89
3	D	336	NAD	N3A-C2A-N1A	-8.25	122.58	128.89
3	C	336	NAD	C4B-O4B-C1B	-3.35	106.04	109.72
3	Q	336	NAD	C4A-C5A-N7A	-3.21	106.53	109.48
3	B	336	NAD	C4A-C5A-N7A	-3.15	106.58	109.48
3	R	336	NAD	C4A-C5A-N7A	-3.01	106.71	109.48
3	C	336	NAD	C4A-C5A-N7A	-2.91	106.81	109.48
3	P	336	NAD	C4B-O4B-C1B	-2.87	106.56	109.72
3	O	336	NAD	C4A-C5A-N7A	-2.86	106.84	109.48
3	A	336	NAD	C4A-C5A-N7A	-2.80	106.90	109.48
3	D	336	NAD	C4B-O4B-C1B	-2.79	106.65	109.72
3	D	336	NAD	C4A-C5A-N7A	-2.68	107.01	109.48
3	O	336	NAD	C4B-O4B-C1B	-2.64	106.82	109.72
3	P	336	NAD	C4A-C5A-N7A	-2.60	107.09	109.48
3	P	336	NAD	O4D-C1D-N1N	-2.57	105.30	108.13
3	B	336	NAD	O4D-C1D-N1N	-2.50	105.38	108.13
3	R	336	NAD	C1B-N9A-C4A	-2.48	123.19	126.94
3	C	336	NAD	C4D-O4D-C1D	-2.35	107.14	109.72
3	A	336	NAD	C4B-O4B-C1B	-2.32	107.17	109.72
3	B	336	NAD	O3-PN-O5D	-2.22	97.04	102.94
3	A	336	NAD	C3N-C7N-N7N	-2.20	115.41	117.82
3	P	336	NAD	C1B-N9A-C4A	-2.17	123.67	126.94
3	Q	336	NAD	O4D-C1D-N1N	-2.17	105.75	108.13
3	P	336	NAD	C4D-O4D-C1D	-2.17	107.34	109.72
3	O	336	NAD	C4D-O4D-C1D	-2.15	107.35	109.72
3	B	336	NAD	C4B-O4B-C1B	-2.13	107.38	109.72
3	Q	336	NAD	C1B-N9A-C4A	-2.08	123.81	126.94
3	O	336	NAD	C1B-N9A-C4A	-2.06	123.83	126.94
3	A	336	NAD	C1B-N9A-C4A	-2.02	123.89	126.94
3	B	336	NAD	C1B-N9A-C4A	-2.01	123.90	126.94
3	R	336	NAD	C2N-C3N-C4N	2.04	120.56	118.29
3	A	336	NAD	C2N-C3N-C4N	2.05	120.57	118.29
3	Q	336	NAD	C2N-C3N-C4N	2.21	120.75	118.29
3	P	336	NAD	C2N-C3N-C4N	2.86	121.47	118.29

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

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, 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	A	329/331 (99%)	-0.10	12 (3%) 46 47	8, 12, 19, 22	0
1	B	329/331 (99%)	0.13	17 (5%) 31 28	7, 12, 19, 22	0
1	C	329/331 (99%)	-0.22	1 (0%) 94 94	8, 11, 18, 24	0
1	D	329/331 (99%)	0.06	16 (4%) 33 31	8, 12, 18, 22	0
1	O	329/331 (99%)	-0.02	17 (5%) 31 28	8, 12, 20, 24	0
1	P	329/331 (99%)	-0.33	0 100 100	8, 11, 18, 24	0
1	Q	329/331 (99%)	-0.16	0 100 100	8, 11, 18, 24	0
1	R	329/331 (99%)	-0.11	5 (1%) 76 79	8, 12, 19, 24	0
All	All	2632/2648 (99%)	-0.09	68 (2%) 59 60	7, 12, 19, 24	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	81	PRO	5.8
1	D	66	GLY	5.3
1	A	83	ALA	4.7
1	O	83	ALA	4.3
1	B	107	LEU	4.3
1	B	83	ALA	4.1
1	O	107	LEU	4.1
1	B	1	MET	4.1
1	D	105	ALA	4.0
1	O	111	ALA	3.9
1	O	142	HIS	3.8
1	D	109	GLY	3.8
1	B	139	SER	3.8
1	A	107	LEU	3.8
1	O	80	ILE	3.7
1	D	82	TRP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	83	ALA	3.6
1	D	83	ALA	3.6
1	D	1	MET	3.5
1	A	81	PRO	3.4
1	O	82	TRP	3.3
1	D	61	TYR	3.3
1	R	1	MET	3.3
1	A	109	GLY	3.2
1	B	82	TRP	3.0
1	B	81	PRO	3.0
1	D	85	ALA	3.0
1	D	79	GLU	2.9
1	O	79	GLU	2.8
1	A	1	MET	2.8
1	A	108	GLU	2.8
1	O	61	TYR	2.8
1	B	80	ILE	2.8
1	B	109	GLY	2.7
1	O	62	LEU	2.7
1	B	85	ALA	2.7
1	O	108	GLU	2.6
1	B	61	TYR	2.6
1	O	109	GLY	2.6
1	D	107	LEU	2.6
1	R	81	PRO	2.6
1	D	59	ASP	2.6
1	O	85	ALA	2.6
1	A	61	TYR	2.6
1	O	1	MET	2.5
1	A	111	ALA	2.5
1	B	28	LEU	2.5
1	A	82	TRP	2.5
1	B	110	GLY	2.4
1	R	109	GLY	2.4
1	O	87	VAL	2.4
1	O	2	LYS	2.4
1	B	111	ALA	2.4
1	D	99	ASP	2.3
1	B	66	GLY	2.3
1	D	81	PRO	2.3
1	R	107	LEU	2.3
1	A	85	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	87	VAL	2.3
1	C	108	GLU	2.2
1	B	108	GLU	2.2
1	A	70	ARG	2.2
1	O	101	ASP	2.1
1	D	111	ALA	2.1
1	A	79	GLU	2.1
1	D	62	LEU	2.1
1	B	101	ASP	2.0
1	B	86	GLY	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	D	149	8/9	0.95	0.09	-	10,11,17,18	0
1	CSD	B	149	8/9	0.97	0.07	-	11,12,15,18	0
1	CSD	Q	149	8/9	0.97	0.08	-	10,11,16,18	0
1	CSD	C	149	8/9	0.97	0.07	-	10,11,16,19	0
1	CSD	O	149	8/9	0.97	0.07	-	11,12,18,19	0
1	CSD	P	149	8/9	0.96	0.08	-	10,11,17,20	0
1	CSD	R	149	8/9	0.97	0.08	-	10,11,17,19	0
1	CSD	A	149	8/9	0.96	0.09	-	11,11,17,18	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	Q	3503	6/6	0.55	0.27	12.83	45,46,48,48	0
4	PGE	C	1700	10/10	0.62	0.20	11.91	26,29,30,31	0
6	GOL	D	3504	6/6	0.66	0.24	11.05	45,46,46,47	0
6	GOL	R	3502	6/6	0.59	0.25	8.32	49,50,50,51	0
5	IPA	Q	1801	4/4	0.76	0.19	5.91	34,35,35,35	0
3	NAD	D	336	44/44	0.96	0.16	3.01	8,10,12,12	0
3	NAD	B	336	44/44	0.98	0.12	2.46	8,10,12,13	0
5	IPA	C	1800	4/4	0.90	0.11	2.12	26,27,27,28	0
3	NAD	A	336	44/44	0.97	0.13	2.11	9,10,12,12	0
3	NAD	O	336	44/44	0.96	0.13	1.14	10,12,13,13	0
3	NAD	R	336	44/44	0.98	0.09	0.96	8,10,11,12	0
3	NAD	C	336	44/44	0.98	0.06	-1.04	9,10,11,13	0
3	NAD	P	336	44/44	0.98	0.05	-2.00	8,9,11,12	0
3	NAD	Q	336	44/44	0.98	0.05	-2.06	8,10,11,12	0
2	NA	C	1600	1/1	0.99	0.06	-	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.