



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 PM GMT

PDB ID : 3RHH
Title : Crystal structure of NADP-dependent glyceraldehyde-3-phosphate dehydrogenase from *Bacillus halodurans* C-125 complexed with NADP
Authors : Malashkevich, V.N.; Toro, R.; Seidel, R.; Garrett, S.; Foti, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-04-11
Resolution : 2.30 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

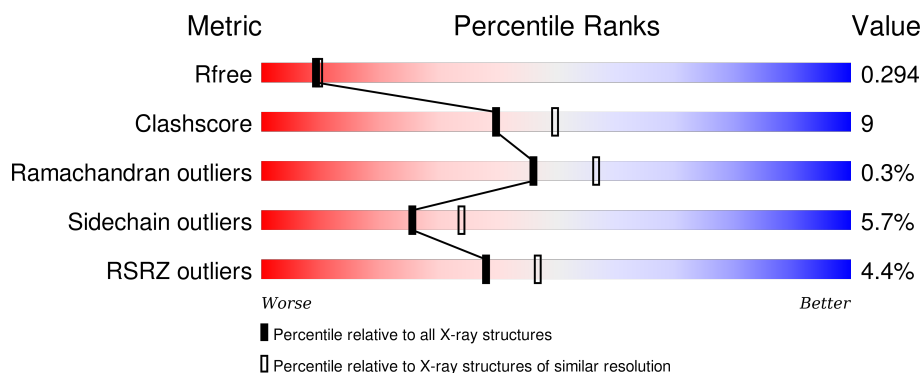
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


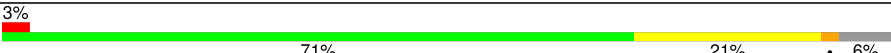
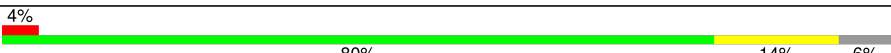

The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	505	 4% 72% 20% • 6%
1	B	505	 3% 71% 21% • 6%
1	C	505	 4% 80% 14% 6%
1	D	505	 6% 72% 21% • 5%

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
2	NAP	A	506	-	-	-	X
2	NAP	D	506	-	-	-	X
3	SO4	D	507	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14718 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 NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3573	2251	621	694	7			
1	B	476	Total	C	N	O	S	0	0	0
			3578	2254	622	695	7			
1	C	476	Total	C	N	O	S	0	2	0
			3594	2265	623	699	7			
1	D	480	Total	C	N	O	S	0	1	0
			3624	2286	627	704	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9KAAQ0
A	2	VAL	-	EXPRESSION TAG	UNP Q9KAAQ0
A	484	ALA	-	EXPRESSION TAG	UNP Q9KAAQ0
A	485	GLU	-	EXPRESSION TAG	UNP Q9KAAQ0
A	486	ASN	-	EXPRESSION TAG	UNP Q9KAAQ0
A	487	LEU	-	EXPRESSION TAG	UNP Q9KAAQ0
A	488	TYR	-	EXPRESSION TAG	UNP Q9KAAQ0
A	489	PHE	-	EXPRESSION TAG	UNP Q9KAAQ0
A	490	GLN	-	EXPRESSION TAG	UNP Q9KAAQ0
A	491	SER	-	EXPRESSION TAG	UNP Q9KAAQ0
A	492	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	493	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	494	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	495	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	496	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	497	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	498	TRP	-	EXPRESSION TAG	UNP Q9KAAQ0
A	499	SER	-	EXPRESSION TAG	UNP Q9KAAQ0
A	500	HIS	-	EXPRESSION TAG	UNP Q9KAAQ0
A	501	PRO	-	EXPRESSION TAG	UNP Q9KAAQ0
A	502	GLN	-	EXPRESSION TAG	UNP Q9KAAQ0

Continued on next page...

Continued from previous page...

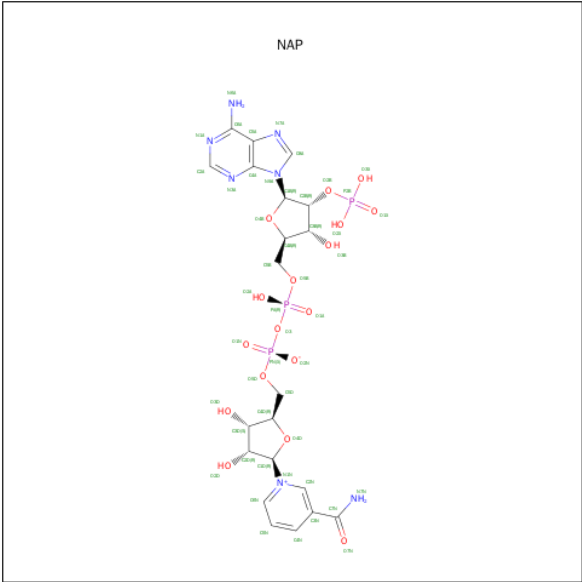
Chain	Residue	Modelled	Actual	Comment	Reference
A	503	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
A	504	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
A	505	LYS	-	EXPRESSION TAG	UNP Q9KAQ0
B	1	MET	-	EXPRESSION TAG	UNP Q9KAQ0
B	2	VAL	-	EXPRESSION TAG	UNP Q9KAQ0
B	484	ALA	-	EXPRESSION TAG	UNP Q9KAQ0
B	485	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
B	486	ASN	-	EXPRESSION TAG	UNP Q9KAQ0
B	487	LEU	-	EXPRESSION TAG	UNP Q9KAQ0
B	488	TYR	-	EXPRESSION TAG	UNP Q9KAQ0
B	489	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
B	490	GLN	-	EXPRESSION TAG	UNP Q9KAQ0
B	491	SER	-	EXPRESSION TAG	UNP Q9KAQ0
B	492	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	493	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	494	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	495	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	496	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	497	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	498	TRP	-	EXPRESSION TAG	UNP Q9KAQ0
B	499	SER	-	EXPRESSION TAG	UNP Q9KAQ0
B	500	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
B	501	PRO	-	EXPRESSION TAG	UNP Q9KAQ0
B	502	GLN	-	EXPRESSION TAG	UNP Q9KAQ0
B	503	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
B	504	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
B	505	LYS	-	EXPRESSION TAG	UNP Q9KAQ0
C	1	MET	-	EXPRESSION TAG	UNP Q9KAQ0
C	2	VAL	-	EXPRESSION TAG	UNP Q9KAQ0
C	484	ALA	-	EXPRESSION TAG	UNP Q9KAQ0
C	485	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
C	486	ASN	-	EXPRESSION TAG	UNP Q9KAQ0
C	487	LEU	-	EXPRESSION TAG	UNP Q9KAQ0
C	488	TYR	-	EXPRESSION TAG	UNP Q9KAQ0
C	489	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
C	490	GLN	-	EXPRESSION TAG	UNP Q9KAQ0
C	491	SER	-	EXPRESSION TAG	UNP Q9KAQ0
C	492	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
C	493	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
C	494	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
C	495	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
C	496	HIS	-	EXPRESSION TAG	UNP Q9KAQ0

Continued on next page...

Continued from previous page...

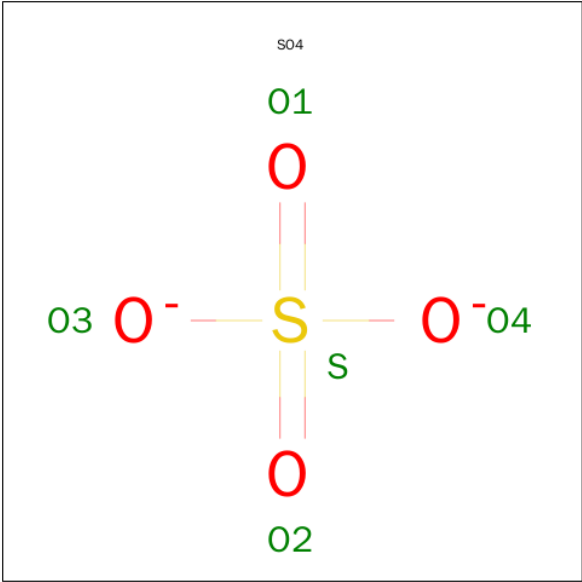
Chain	Residue	Modelled	Actual	Comment	Reference
C	497	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
C	498	TRP	-	EXPRESSION TAG	UNP Q9KAQ0
C	499	SER	-	EXPRESSION TAG	UNP Q9KAQ0
C	500	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
C	501	PRO	-	EXPRESSION TAG	UNP Q9KAQ0
C	502	GLN	-	EXPRESSION TAG	UNP Q9KAQ0
C	503	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
C	504	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
C	505	LYS	-	EXPRESSION TAG	UNP Q9KAQ0
D	1	MET	-	EXPRESSION TAG	UNP Q9KAQ0
D	2	VAL	-	EXPRESSION TAG	UNP Q9KAQ0
D	484	ALA	-	EXPRESSION TAG	UNP Q9KAQ0
D	485	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
D	486	ASN	-	EXPRESSION TAG	UNP Q9KAQ0
D	487	LEU	-	EXPRESSION TAG	UNP Q9KAQ0
D	488	TYR	-	EXPRESSION TAG	UNP Q9KAQ0
D	489	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
D	490	GLN	-	EXPRESSION TAG	UNP Q9KAQ0
D	491	SER	-	EXPRESSION TAG	UNP Q9KAQ0
D	492	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	493	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	494	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	495	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	496	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	497	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	498	TRP	-	EXPRESSION TAG	UNP Q9KAQ0
D	499	SER	-	EXPRESSION TAG	UNP Q9KAQ0
D	500	HIS	-	EXPRESSION TAG	UNP Q9KAQ0
D	501	PRO	-	EXPRESSION TAG	UNP Q9KAQ0
D	502	GLN	-	EXPRESSION TAG	UNP Q9KAQ0
D	503	PHE	-	EXPRESSION TAG	UNP Q9KAQ0
D	504	GLU	-	EXPRESSION TAG	UNP Q9KAQ0
D	505	LYS	-	EXPRESSION TAG	UNP Q9KAQ0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

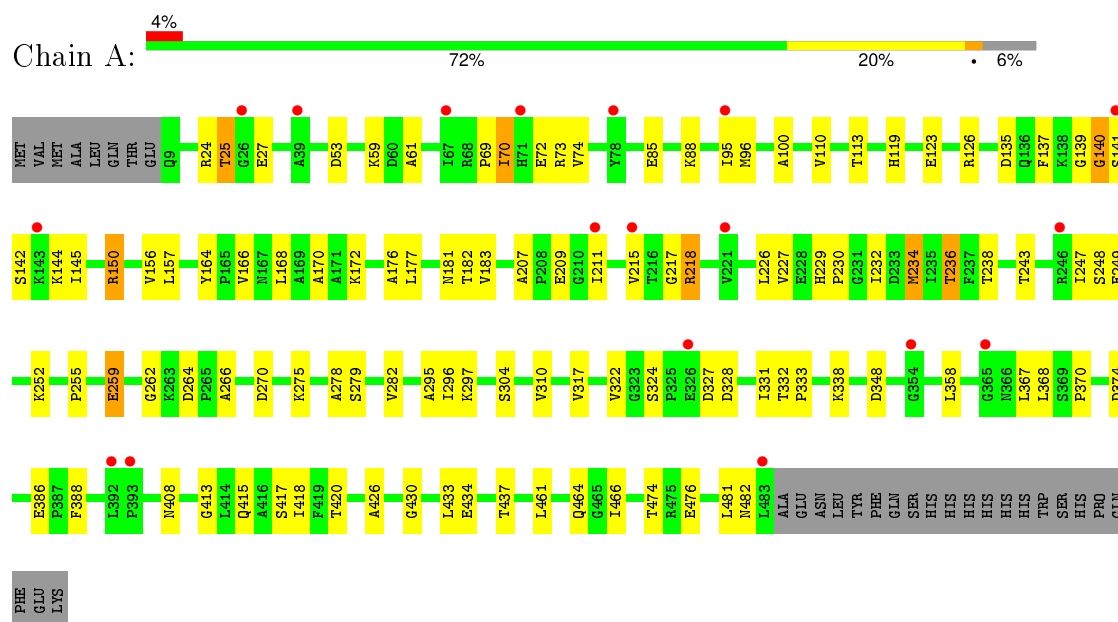
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	60	Total O 60 60	0	0
4	B	65	Total O 65 65	0	0
4	C	37	Total O 37 37	0	0
4	D	43	Total O 43 43	0	0

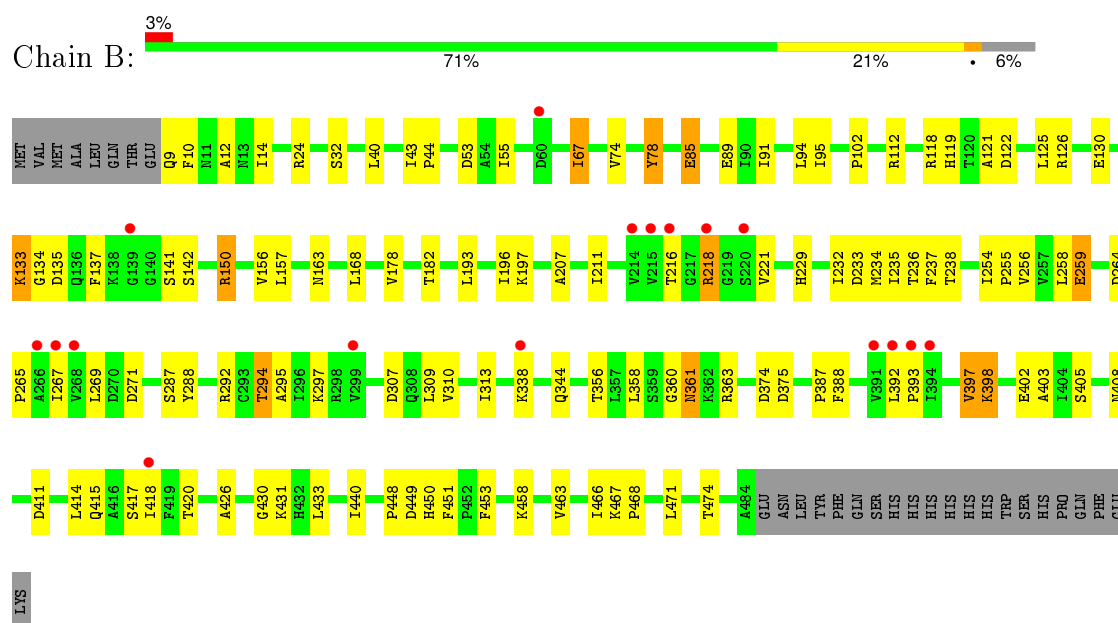
3 Residue-property plots [i](#)

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.

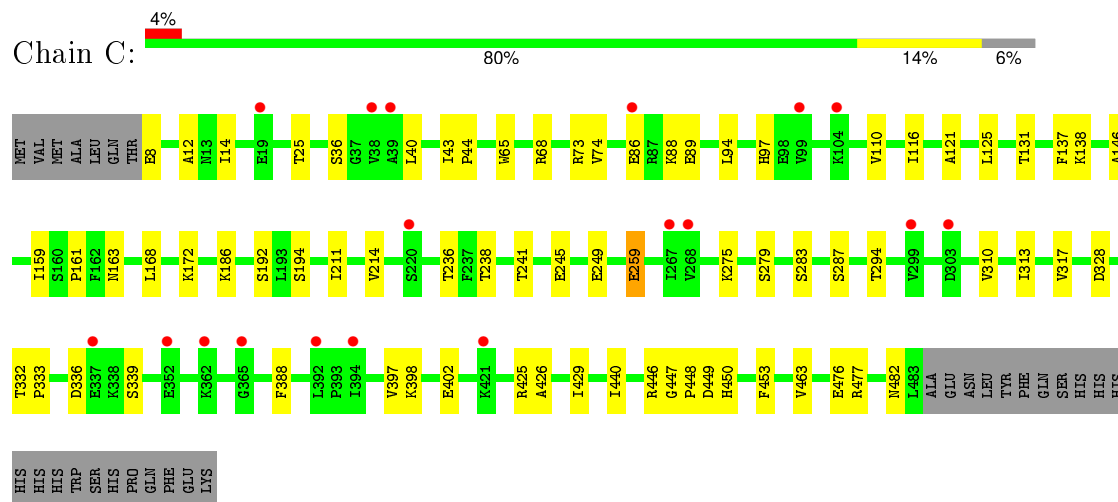
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



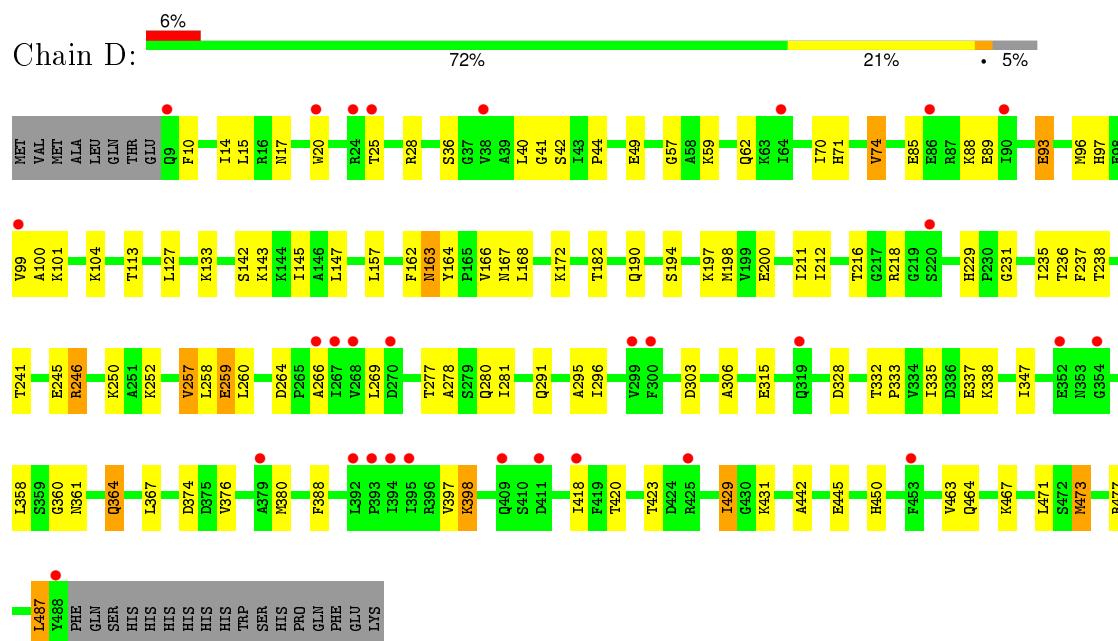
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.65Å 130.75Å 86.92Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-2.30) 95.3 (19.91-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.232 , 0.297 0.233 , 0.294	Depositor DCC
R_{free} test set	3880 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.7	EDS
Estimated twinning fraction	0.030 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77847 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14718	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.59% 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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.46	0/3627	0.62	0/4919
1	B	0.54	1/3632 (0.0%)	0.64	0/4926
1	C	0.44	0/3654	0.60	0/4955
1	D	0.47	0/3683	0.61	0/4996
All	All	0.48	1/14596 (0.0%)	0.62	0/19796

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	TYR	CD1-CE1	-5.17	1.31	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3573	0	3656	69	0
1	B	3578	0	3661	83	0
1	C	3594	0	3681	43	0
1	D	3624	0	3702	75	0
2	A	31	0	11	2	0
2	B	31	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	11	0	0
2	D	31	0	11	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
4	A	60	0	0	3	0
4	B	65	0	0	8	0
4	C	37	0	0	2	0
4	D	43	0	0	4	0
All	All	14718	0	14744	256	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 9.

All (256) 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:B:238:THR:HG23	1:B:259:GLU:HG3	1.48	0.95
1:D:257:VAL:O	1:D:257:VAL:HG12	1.64	0.94
1:B:218:ARG:HG3	1:B:221:VAL:HB	1.52	0.91
1:D:259:GLU:CD	1:D:464:GLN:HE22	1.75	0.90
1:B:294:THR:HG22	1:B:414:LEU:HD21	1.54	0.88
1:D:266:ALA:HB2	1:D:296:ILE:HD13	1.57	0.86
1:B:207:ALA:HB1	1:B:211:ILE:HD11	1.58	0.85
1:A:259:GLU:HB3	1:A:464:GLN:HE22	1.46	0.81
1:B:397:VAL:HG22	1:B:402:GLU:HB3	1.61	0.80
1:B:238:THR:HG23	1:B:259:GLU:CG	2.12	0.80
1:B:236:THR:HG21	4:B:559:HOH:O	1.82	0.77
1:C:447:GLY:HA3	4:C:523:HOH:O	1.86	0.75
1:A:156:VAL:HG13	1:A:234:MET:HE2	1.70	0.73
1:A:156:VAL:HG13	1:A:234:MET:CE	2.19	0.72
1:D:257:VAL:O	1:D:257:VAL:CG1	2.30	0.72
1:D:229:HIS:HD2	1:D:231:GLY:H	1.35	0.72
1:D:277:THR:O	1:D:281:ILE:HG12	1.90	0.71
1:C:74:VAL:HG21	1:C:125:LEU:HD13	1.72	0.71
1:D:113:THR:OG1	1:D:167:ASN:HA	1.90	0.71
1:D:163:ASN:ND2	1:D:291:GLN:O	2.23	0.71
1:D:182:THR:HG22	1:D:211:ILE:HA	1.75	0.69
1:A:211:ILE:HB	4:A:517:HOH:O	1.93	0.68
1:D:96:MET:O	1:D:100:ALA:HA	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:GLY:O	1:C:477:ARG:NH2	2.26	0.68
1:D:10:PHE:O	1:D:41:GLY:HA3	1.94	0.68
1:B:156:VAL:HG13	1:B:234:MET:CE	2.24	0.68
1:A:418:ILE:HD11	1:A:433:LEU:HD11	1.75	0.68
1:A:141:SER:HB3	1:A:144:LYS:HE2	1.76	0.67
1:D:259:GLU:CD	1:D:464:GLN:NE2	2.46	0.67
1:D:40:LEU:HD11	1:D:97:HIS:HB3	1.76	0.67
1:C:238:THR:HG23	1:C:259:GLU:CG	2.24	0.67
1:A:332:THR:HB	1:A:333:PRO:HD2	1.76	0.67
1:D:264:ASP:HB2	1:D:295:ALA:O	1.95	0.66
1:B:218:ARG:HB3	4:B:509:HOH:O	1.95	0.66
1:A:168:LEU:HD13	1:A:238:THR:HG21	1.79	0.65
1:D:259:GLU:CG	1:D:464:GLN:HE22	2.10	0.65
1:A:358:LEU:HD11	1:A:374:ASP:HB2	1.77	0.65
1:B:24:ARG:NH2	1:B:53:ASP:OD2	2.29	0.64
1:B:130:GLU:HB3	4:D:527:HOH:O	1.98	0.64
1:A:70:ILE:HD12	1:A:73:ARG:NH2	2.14	0.63
1:C:172[B]:LYS:NZ	1:C:238:THR:OG1	2.25	0.62
1:A:264:ASP:HB2	1:A:295:ALA:O	2.00	0.62
1:A:207:ALA:HB1	4:A:517:HOH:O	1.99	0.61
1:D:164:TYR:HB3	1:D:167:ASN:HB3	1.80	0.61
1:B:358:LEU:HD11	1:B:374:ASP:HB2	1.82	0.61
1:C:65:TRP:HB2	1:C:211:ILE:HD11	1.82	0.61
1:B:218:ARG:HG3	1:B:221:VAL:CB	2.26	0.61
1:B:264:ASP:HB2	1:B:295:ALA:O	2.01	0.60
1:D:303:ASP:HA	1:D:306:ALA:HB2	1.84	0.60
1:A:420:THR:CG2	1:A:426:ALA:HB2	2.31	0.60
1:C:168:LEU:HD13	1:C:238:THR:HG21	1.84	0.60
1:A:156:VAL:HB	1:A:183:VAL:HG22	1.83	0.60
1:D:347:ILE:HG21	1:D:361:ASN:OD1	2.03	0.59
1:D:237:PHE:HB3	1:D:258:LEU:HD23	1.84	0.59
1:D:229:HIS:CD2	1:D:231:GLY:H	2.19	0.58
1:B:271:ASP:OD1	1:B:420:THR:OG1	2.20	0.58
1:D:133:LYS:HD3	1:D:145:ILE:HD12	1.84	0.58
1:A:182:THR:HG22	1:A:211:ILE:HA	1.86	0.57
1:D:376:VAL:HA	1:D:380:MET:SD	2.44	0.57
1:D:236:THR:HA	1:D:257:VAL:HG12	1.86	0.57
1:B:137:PHE:HB2	1:C:450:HIS:ND1	2.19	0.57
1:C:259:GLU:HG3	1:C:259:GLU:O	2.04	0.57
1:B:78:TYR:OH	1:B:122:ASP:OD2	2.23	0.57
1:A:61:ALA:HB1	1:A:211:ILE:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:THR:HA	1:C:146:ALA:O	2.05	0.56
1:B:411:ASP:HB3	1:B:458:LYS:HG3	1.86	0.56
1:D:59:LYS:HE3	4:D:514:HOH:O	2.05	0.56
1:B:463:VAL:HG21	1:C:476:GLU:OE1	2.07	0.55
1:B:267:ILE:HG12	1:B:403:ALA:HB1	1.88	0.55
1:C:172[A]:LYS:HD3	1:C:236:THR:HB	1.89	0.55
1:C:43:ILE:HG21	1:C:192:SER:HB2	1.89	0.55
1:D:418:ILE:CD1	1:D:429:ILE:HG22	2.36	0.55
1:B:134:GLY:HA3	1:B:141:SER:O	2.07	0.55
1:C:259:GLU:OE1	1:C:446:ARG:NH2	2.39	0.55
1:C:238:THR:HG23	1:C:259:GLU:HG2	1.88	0.55
1:A:317:VAL:HG13	1:A:370:PRO:HB2	1.88	0.55
1:B:287:SER:HB2	1:B:292:ARG:HH11	1.72	0.55
1:B:157:LEU:HD23	1:B:235:ILE:HG12	1.89	0.55
1:B:310:VAL:CG1	1:B:358:LEU:HD13	2.37	0.55
1:A:415:GLN:HG2	1:A:437:THR:HB	1.88	0.54
1:D:157:LEU:HD23	1:D:235:ILE:CD1	2.38	0.54
1:B:408:ASN:HB3	4:B:532:HOH:O	2.07	0.54
1:B:119:HIS:HD2	1:B:466:ILE:HG21	1.73	0.54
1:B:156:VAL:HG13	1:B:234:MET:HE1	1.88	0.54
1:B:12:ALA:HB1	1:B:196:ILE:HD13	1.90	0.54
4:B:515:HOH:O	1:C:482:ASN:HB2	2.08	0.54
1:A:145:ILE:HD11	1:A:481:LEU:HD12	1.89	0.54
1:D:70:ILE:O	1:D:74:VAL:HG13	2.07	0.54
1:B:182:THR:CG2	1:B:211:ILE:HA	2.38	0.53
1:C:425:ARG:HE	1:D:487:LEU:HD13	1.73	0.53
1:A:249:GLU:HB2	1:D:252:LYS:HD3	1.90	0.53
1:B:450:HIS:ND1	1:C:137:PHE:HB2	2.24	0.53
1:D:10:PHE:N	1:D:40:LEU:O	2.42	0.53
1:B:356:THR:OG1	1:B:375:ASP:OD2	2.25	0.53
1:D:166:VAL:HG13	1:D:198:MET:HG3	1.89	0.53
1:A:88:LYS:HA	1:A:110:VAL:HG11	1.91	0.53
1:B:168:LEU:HD13	1:B:238:THR:HG21	1.91	0.52
1:B:182:THR:HG22	1:B:211:ILE:HA	1.90	0.52
1:D:358:LEU:HD11	1:D:374:ASP:HB2	1.92	0.52
1:D:241:THR:HA	1:D:260:LEU:HD22	1.90	0.52
1:B:156:VAL:HG13	1:B:234:MET:HE2	1.91	0.51
1:B:449:ASP:O	1:B:466:ILE:HG12	2.11	0.51
1:A:266:ALA:HB2	1:A:296:ILE:HD12	1.93	0.51
1:D:182:THR:CG2	1:D:211:ILE:HA	2.41	0.51
1:D:246:ARG:O	1:D:250:LYS:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:HE3	1:B:142:SER:O	2.11	0.50
1:A:156:VAL:HG21	1:A:176:ALA:HB1	1.94	0.50
1:D:418:ILE:HD13	1:D:429:ILE:HG22	1.93	0.50
1:B:150:ARG:HD3	1:B:474:THR:OG1	2.12	0.50
1:D:278:ALA:HB3	4:D:531:HOH:O	2.11	0.49
1:D:259:GLU:CG	1:D:464:GLN:NE2	2.73	0.49
1:A:70:ILE:O	1:A:74:VAL:HG13	2.13	0.49
1:A:164:TYR:HB2	1:A:168:LEU:HD12	1.94	0.49
1:A:119:HIS:HD2	1:A:466:ILE:HG21	1.77	0.49
1:B:43:ILE:HD12	1:B:216:THR:HB	1.95	0.49
1:B:398:LYS:HB2	1:B:402:GLU:OE1	2.13	0.49
1:C:426:ALA:HB1	1:C:440:ILE:HD12	1.95	0.49
1:D:280:GLN:OE1	1:D:442:ALA:HA	2.13	0.49
1:B:294:THR:HG22	1:B:414:LEU:CD2	2.36	0.49
1:B:163:ASN:HB2	1:B:288:TYR:HE2	1.78	0.49
1:B:259:GLU:O	1:B:259:GLU:HG3	2.11	0.48
1:B:112:ARG:NH1	3:B:507:SO4:O4	2.38	0.48
1:D:259:GLU:OE2	1:D:464:GLN:OE1	2.31	0.48
1:D:93:GLU:HA	1:D:96:MET:HG2	1.94	0.48
1:C:241:THR:O	1:C:245:GLU:HG3	2.14	0.48
1:B:417:SER:O	1:B:418:ILE:HD13	2.13	0.48
1:C:332:THR:HB	1:C:333:PRO:CD	2.43	0.48
1:D:99:VAL:HG11	1:D:162:PHE:O	2.14	0.48
1:A:95:ILE:HD11	1:A:166:VAL:CG2	2.44	0.47
1:C:116:ILE:HD11	1:C:449:ASP:OD1	2.14	0.47
1:D:190:GLN:HG2	1:D:335:ILE:HD11	1.96	0.47
1:A:157:LEU:HB2	1:A:232:ILE:HD12	1.95	0.47
1:B:135:ASP:HB2	1:D:71:HIS:HB3	1.95	0.47
1:A:227:VAL:HG21	1:A:247:ILE:HG12	1.97	0.47
1:D:17:ASN:OD1	1:D:57:GLY:HA3	2.14	0.47
1:A:137:PHE:HB2	1:D:450:HIS:ND1	2.30	0.47
1:A:430:GLY:O	1:D:477:ARG:NH2	2.48	0.47
1:D:85:GLU:O	1:D:88:LYS:HG2	2.15	0.47
1:D:246:ARG:HH11	1:D:250:LYS:HZ3	1.62	0.46
1:A:172:LYS:HG2	1:A:236:THR:HG21	1.97	0.46
1:D:104:LYS:HG3	4:D:550:HOH:O	2.15	0.46
1:B:102:PRO:HB2	4:B:550:HOH:O	2.15	0.46
1:A:172:LYS:HD3	1:A:236:THR:HB	1.98	0.46
1:C:14:ILE:HD13	1:C:214:VAL:O	2.15	0.46
1:B:338:LYS:HG3	4:B:524:HOH:O	2.16	0.46
1:D:28:ARG:HH22	1:D:44:PRO:HD3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:HH11	1:D:250:LYS:NZ	2.13	0.46
1:C:74:VAL:HG13	1:C:121:ALA:HB1	1.97	0.45
1:B:448:PRO:HD2	1:B:451:PHE:CD2	2.51	0.45
1:A:408:ASN:CG	1:A:434:GLU:HG3	2.37	0.45
1:A:278:ALA:O	1:A:282:VAL:HG23	2.16	0.45
1:D:197:LYS:HA	1:D:197:LYS:HD3	1.84	0.45
1:B:237:PHE:HB3	1:B:258:LEU:HD23	1.99	0.45
1:A:176:ALA:O	1:A:181:ASN:HB2	2.17	0.45
1:C:429:ILE:HG12	1:D:487:LEU:HD22	1.99	0.45
1:A:322:VAL:HB	1:A:331:ILE:HB	1.97	0.45
1:A:150:ARG:HG2	1:A:474:THR:HB	1.99	0.45
1:A:177:LEU:HD22	1:A:211:ILE:HG22	1.99	0.45
1:B:85:GLU:OE2	1:B:118:ARG:NH2	2.47	0.45
1:C:86:GLU:HB2	4:C:533:HOH:O	2.15	0.45
1:B:310:VAL:HG11	1:B:358:LEU:CD1	2.47	0.45
1:A:229:HIS:HA	1:A:230:PRO:HD3	1.88	0.45
1:B:91:ILE:O	1:B:95:ILE:HG13	2.17	0.45
1:C:336:ASP:O	1:C:339:SER:HB3	2.17	0.45
1:D:14:ILE:HG21	1:D:216:THR:OG1	2.17	0.45
1:D:333:PRO:HD3	1:D:367:LEU:HD13	1.98	0.44
1:B:67:ILE:HA	1:B:67:ILE:HD13	1.83	0.44
1:B:398:LYS:HE3	1:B:398:LYS:HB3	1.42	0.44
1:B:418:ILE:HD11	1:B:433:LEU:HD11	1.99	0.44
1:B:361:ASN:O	1:B:361:ASN:CG	2.55	0.44
1:C:313:ILE:O	1:C:317:VAL:HG23	2.18	0.44
1:B:218:ARG:HA	4:B:509:HOH:O	2.16	0.44
1:B:233:ASP:O	1:B:255:PRO:HD2	2.17	0.44
1:D:164:TYR:HB2	1:D:168:LEU:HD12	1.99	0.44
1:D:157:LEU:HD23	1:D:235:ILE:HD13	1.98	0.44
1:D:172:LYS:O	1:D:473:MET:HE1	2.18	0.44
1:B:310:VAL:CG1	1:B:358:LEU:CD1	2.95	0.44
1:A:420:THR:HG22	1:A:426:ALA:HB2	1.99	0.44
1:A:322:VAL:HG23	1:A:367:LEU:HD21	1.99	0.44
1:A:215:VAL:HG21	1:A:226:LEU:HD21	1.99	0.44
1:A:234:MET:HG3	1:A:255:PRO:HB2	2.00	0.44
1:C:259:GLU:CD	1:C:453:PHE:HE2	2.21	0.44
1:D:163:ASN:HA	1:D:163:ASN:HD22	1.60	0.43
1:B:232:ILE:O	1:B:254:ILE:HG21	2.18	0.43
1:C:447:GLY:CA	1:C:448:PRO:C	2.87	0.43
1:A:182:THR:CG2	1:A:211:ILE:HA	2.47	0.43
1:A:275:LYS:HD3	1:A:275:LYS:HA	1.88	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PRO:HG2	1:A:72:GLU:HG3	2.00	0.43
1:B:297:LYS:O	1:B:393:PRO:HD2	2.19	0.43
1:C:275:LYS:O	1:C:279:SER:HB2	2.19	0.43
1:B:294:THR:HG21	1:B:453:PHE:CE1	2.54	0.43
1:B:74:VAL:HG21	1:B:125:LEU:HD13	1.99	0.43
1:A:476:GLU:OE1	1:D:463:VAL:HG21	2.18	0.43
1:B:218:ARG:HG3	1:B:221:VAL:CG2	2.48	0.43
1:A:297:LYS:NZ	1:A:386:GLU:OE2	2.48	0.43
1:B:74:VAL:HG13	1:B:121:ALA:HB1	2.00	0.43
1:A:113:THR:HG23	1:A:170:ALA:HB3	2.01	0.43
1:B:420:THR:HG22	1:B:426:ALA:HB2	2.00	0.43
1:D:96:MET:CB	1:D:101:LYS:O	2.67	0.42
1:B:287:SER:HB2	1:B:292:ARG:NH1	2.33	0.42
1:A:238:THR:HG23	1:A:259:GLU:HG3	2.01	0.42
1:D:28:ARG:HD3	1:D:42:SER:OG	2.20	0.42
1:A:262:GLY:O	1:A:297:LYS:HD2	2.19	0.42
1:B:10:PHE:CD1	1:B:193:LEU:HD22	2.55	0.42
1:B:9:GLN:HB2	1:B:40:LEU:O	2.20	0.42
1:A:123:GLU:HG2	1:B:126:ARG:HE	1.85	0.42
1:A:243:THR:HG1	2:A:506:NAP:PA	2.42	0.42
1:C:12:ALA:O	1:C:44:PRO:HD3	2.20	0.42
1:C:68:ARG:O	1:C:73:ARG:NH1	2.53	0.42
1:A:217:GLY:O	1:A:218:ARG:C	2.57	0.42
1:A:348:ASP:HB2	4:A:523:HOH:O	2.19	0.42
1:D:397:VAL:HG12	1:D:398:LYS:N	2.34	0.42
1:B:344:GLN:OE1	1:B:363:ARG:HD2	2.20	0.41
1:B:55:ILE:HD13	1:B:229:HIS:CG	2.55	0.41
1:C:397:VAL:HG22	1:C:402:GLU:HB3	2.01	0.41
1:C:40:LEU:HD11	1:C:97:HIS:HB3	2.02	0.41
1:B:426:ALA:HB1	1:B:440:ILE:HD12	2.02	0.41
1:A:85:GLU:O	1:A:88:LYS:HG2	2.19	0.41
1:D:127:LEU:HA	1:D:127:LEU:HD23	1.91	0.41
1:C:88:LYS:HA	1:C:110:VAL:HG11	2.02	0.41
1:D:418:ILE:HD13	1:D:429:ILE:CG2	2.49	0.41
1:B:297:LYS:HD3	1:B:387:PRO:HD2	2.02	0.41
1:A:243:THR:HB	2:A:506:NAP:O2A	2.20	0.41
1:A:24:ARG:NH2	1:A:53:ASP:OD2	2.48	0.41
1:D:238:THR:HA	1:D:259:GLU:O	2.19	0.41
1:A:177:LEU:HD22	1:A:211:ILE:CG2	2.51	0.41
1:C:172[B]:LYS:HZ2	1:C:236:THR:HG22	1.86	0.41
1:C:259:GLU:O	1:C:259:GLU:CG	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:ARG:HG3	1:C:453:PHE:CG	2.55	0.41
1:D:418:ILE:HD11	1:D:429:ILE:HG22	2.01	0.41
1:B:94:LEU:HD23	1:B:197:LYS:HG3	2.02	0.41
1:A:135:ASP:C	1:A:137:PHE:H	2.24	0.41
1:A:324:SER:HB3	1:A:327:ASP:OD2	2.20	0.41
1:D:20:TRP:CZ2	1:D:200:GLU:HA	2.55	0.41
1:D:259:GLU:HG2	1:D:464:GLN:NE2	2.36	0.41
1:B:392:LEU:HD12	1:B:393:PRO:HD2	2.02	0.41
1:C:159:ILE:HA	1:C:186:LYS:O	2.20	0.41
1:D:236:THR:OG1	1:D:257:VAL:HG11	2.20	0.41
1:A:248:SER:OG	1:D:252:LYS:HB2	2.21	0.41
1:B:309:LEU:O	1:B:313:ILE:HG13	2.21	0.41
1:D:445:GLU:HB2	3:D:507:SO4:O3	2.21	0.41
1:B:265:PRO:HD2	1:B:415:GLN:O	2.20	0.41
1:B:218:ARG:HG2	1:B:218:ARG:H	1.34	0.41
1:A:96:MET:O	1:A:100:ALA:HA	2.21	0.41
1:D:15:LEU:HD21	1:D:212:ILE:HG23	2.02	0.41
1:A:417:SER:O	1:A:418:ILE:HD13	2.20	0.40
4:B:515:HOH:O	1:C:482:ASN:CB	2.68	0.40
1:B:14:ILE:HG13	1:B:44:PRO:HG2	2.02	0.40
1:A:139:GLY:O	1:A:140:GLY:C	2.60	0.40
1:C:259:GLU:OE1	1:C:453:PHE:HE2	2.05	0.40
1:D:364:GLN:N	1:D:367:LEU:O	2.50	0.40
1:A:126:ARG:HD2	1:B:126:ARG:HD3	2.03	0.40
1:A:25:THR:CG2	1:A:27:GLU:HG2	2.52	0.40
1:A:144:LYS:HB3	1:A:482:ASN:OD1	2.20	0.40
1:C:94:LEU:HD23	1:C:194:SER:HA	2.04	0.40
1:B:467:LYS:N	1:B:468:PRO:CD	2.85	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	473/505 (94%)	445 (94%)	25 (5%)	3 (1%)	30	36
1	B	474/505 (94%)	453 (96%)	20 (4%)	1 (0%)	52	64
1	C	476/505 (94%)	453 (95%)	22 (5%)	1 (0%)	52	64
1	D	479/505 (95%)	456 (95%)	22 (5%)	1 (0%)	52	64
All	All	1902/2020 (94%)	1807 (95%)	89 (5%)	6 (0%)	46	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	GLY
1	A	218	ARG
1	D	360	GLY
1	B	360	GLY
1	C	161	PRO
1	A	413	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	A	386/414 (93%)	367 (95%)	19 (5%)	31	41
1	B	386/414 (93%)	366 (95%)	20 (5%)	29	38
1	C	389/414 (94%)	373 (96%)	16 (4%)	37	50
1	D	391/414 (94%)	357 (91%)	34 (9%)	13	15
All	All	1552/1656 (94%)	1463 (94%)	89 (6%)	25	34

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	59	LYS
1	A	70	ILE
1	A	142	SER
1	A	150	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	209	GLU
1	A	234	MET
1	A	236	THR
1	A	252	LYS
1	A	259	GLU
1	A	270	ASP
1	A	279	SER
1	A	304	SER
1	A	310	VAL
1	A	328	ASP
1	A	338	LYS
1	A	368	LEU
1	A	388	PHE
1	A	461	LEU
1	B	32	SER
1	B	67	ILE
1	B	85	GLU
1	B	89	GLU
1	B	133	LYS
1	B	150	ARG
1	B	178	VAL
1	B	218	ARG
1	B	256	VAL
1	B	259	GLU
1	B	269	LEU
1	B	294	THR
1	B	307	ASP
1	B	361	ASN
1	B	388	PHE
1	B	397	VAL
1	B	398	LYS
1	B	405	SER
1	B	431	LYS
1	B	471	LEU
1	C	8	GLU
1	C	25	THR
1	C	36	SER
1	C	89	GLU
1	C	138	LYS
1	C	163	ASN
1	C	249	GLU
1	C	259	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	283	SER
1	C	287	SER
1	C	294	THR
1	C	310	VAL
1	C	328	ASP
1	C	388	PHE
1	C	398	LYS
1	C	463	VAL
1	D	25	THR
1	D	36	SER
1	D	49	GLU
1	D	62	GLN
1	D	74	VAL
1	D	89	GLU
1	D	93	GLU
1	D	142	SER
1	D	143	LYS
1	D	147	LEU
1	D	163	ASN
1	D	194	SER
1	D	218	ARG
1	D	245	GLU
1	D	246	ARG
1	D	257	VAL
1	D	259	GLU
1	D	269	LEU
1	D	315	GLU
1	D	328	ASP
1	D	332	THR
1	D	337	GLU
1	D	338	LYS
1	D	364	GLN
1	D	388	PHE
1	D	398	LYS
1	D	420	THR
1	D	423	THR
1	D	429	ILE
1	D	431	LYS
1	D	467	LYS
1	D	471	LEU
1	D	473	MET
1	D	487	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	401	ASN
1	A	464	GLN
1	B	119	HIS
1	B	401	ASN
1	C	48	GLN
1	C	163	ASN
1	C	409	GLN
1	C	432	HIS
1	C	464	GLN
1	D	48	GLN
1	D	52	ASN
1	D	62	GLN
1	D	229	HIS
1	D	308	GLN
1	D	366	ASN
1	D	409	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	A	506	-	27,33,52	1.36	3 (11%)	34,52,80	2.17	2 (5%)
3	SO4	A	507	-	4,4,4	0.30	0	6,6,6	0.13	0
2	NAP	B	506	-	27,33,52	1.37	3 (11%)	34,52,80	2.18	1 (2%)
3	SO4	B	507	-	4,4,4	0.22	0	6,6,6	0.23	0
2	NAP	C	506	-	27,33,52	1.37	3 (11%)	34,52,80	2.30	5 (14%)
3	SO4	C	507	-	4,4,4	0.35	0	6,6,6	0.14	0
2	NAP	D	506	-	27,33,52	1.35	3 (11%)	34,52,80	2.22	4 (11%)
3	SO4	D	507	-	4,4,4	0.29	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
2	NAP	A	506	-	-	0/17/37/67	0/3/3/5
3	SO4	A	507	-	-	0/0/0/0	0/0/0/0
2	NAP	B	506	-	-	0/17/37/67	0/3/3/5
3	SO4	B	507	-	-	0/0/0/0	0/0/0/0
2	NAP	C	506	-	-	0/17/37/67	0/3/3/5
3	SO4	C	507	-	-	0/0/0/0	0/0/0/0
2	NAP	D	506	-	-	0/17/37/67	0/3/3/5
3	SO4	D	507	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	506	NAP	C2A-N1A	2.38	1.38	1.33
2	B	506	NAP	C2A-N1A	2.49	1.38	1.33
2	A	506	NAP	C2A-N1A	2.51	1.38	1.33
2	C	506	NAP	C2A-N1A	2.52	1.38	1.33
2	D	506	NAP	C2A-N3A	3.45	1.38	1.32
2	B	506	NAP	C2A-N3A	3.63	1.38	1.32
2	C	506	NAP	C2A-N3A	3.63	1.38	1.32
2	A	506	NAP	C2A-N3A	3.67	1.38	1.32
2	C	506	NAP	PN-O1N	3.68	1.61	1.50
2	A	506	NAP	PN-O1N	3.80	1.62	1.50
2	B	506	NAP	PN-O1N	3.82	1.62	1.50
2	D	506	NAP	PN-O1N	3.84	1.62	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	506	NAP	N3A-C2A-N1A	-11.80	119.86	128.89
2	D	506	NAP	N3A-C2A-N1A	-11.51	120.08	128.89
2	A	506	NAP	N3A-C2A-N1A	-11.15	120.36	128.89
2	B	506	NAP	N3A-C2A-N1A	-11.14	120.36	128.89
2	C	506	NAP	C1B-N9A-C4A	-2.31	123.46	126.94
2	C	506	NAP	O4B-C1B-C2B	-2.17	102.68	106.60
2	D	506	NAP	C4A-C5A-N7A	-2.07	107.58	109.48
2	D	506	NAP	O3B-C3B-C4B	-2.01	105.02	111.05
2	D	506	NAP	O5D-PN-O2N	2.08	119.01	110.61
2	C	506	NAP	O5D-PN-O2N	2.17	119.38	110.61
2	C	506	NAP	C4B-O4B-C1B	2.44	112.40	109.72
2	A	506	NAP	O5D-PN-O2N	2.76	121.75	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	NAP	2	0
3	B	507	SO4	1	0
3	D	507	SO4	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	A	475/505 (94%)	0.34	18 (3%) 44 53	33, 47, 64, 78	0
1	B	476/505 (94%)	0.23	17 (3%) 46 55	22, 45, 60, 68	0
1	C	476/505 (94%)	0.40	18 (3%) 44 53	31, 52, 74, 89	0
1	D	480/505 (95%)	0.49	30 (6%) 23 31	33, 56, 74, 90	0
All	All	1907/2020 (94%)	0.37	83 (4%) 38 47	22, 49, 70, 90	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	394	ILE	5.4
1	D	220	SER	4.6
1	D	268	VAL	4.3
1	D	299	VAL	4.3
1	C	299	VAL	3.9
1	C	99	VAL	3.8
1	A	143	LYS	3.6
1	D	38	VAL	3.5
1	D	266	ALA	3.5
1	D	90	ILE	3.4
1	D	20	TRP	3.3
1	A	354	GLY	3.3
1	B	392	LEU	3.3
1	D	425	ARG	3.3
1	D	64	ILE	3.2
1	A	141	SER	3.1
1	B	220	SER	3.1
1	D	393	PRO	3.1
1	C	39	ALA	3.0
1	B	393	PRO	3.0
1	B	299	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	267	ILE	2.9
1	D	267	ILE	2.9
1	B	139	GLY	2.8
1	C	220	SER	2.8
1	A	39	ALA	2.8
1	D	395	ILE	2.7
1	A	67	ILE	2.7
1	C	19	GLU	2.7
1	C	394	ILE	2.7
1	D	300	PHE	2.6
1	C	392	LEU	2.6
1	D	379	ALA	2.6
1	D	99	VAL	2.6
1	D	409	GLN	2.6
1	A	221	VAL	2.6
1	C	104	LYS	2.5
1	A	215	VAL	2.5
1	C	38	VAL	2.5
1	A	211	ILE	2.5
1	A	26	GLY	2.5
1	B	391	VAL	2.5
1	D	270	ASP	2.5
1	D	354	GLY	2.5
1	D	86	GLU	2.5
1	C	337	GLU	2.4
1	D	352	GLU	2.4
1	B	268	VAL	2.4
1	C	362	LYS	2.4
1	C	352	GLU	2.4
1	C	268	VAL	2.4
1	B	60	ASP	2.3
1	A	392	LEU	2.3
1	B	267	ILE	2.3
1	B	338	LYS	2.3
1	D	453	PHE	2.3
1	B	216	THR	2.3
1	D	24	ARG	2.2
1	A	483	LEU	2.2
1	A	365	GLY	2.2
1	C	303	ASP	2.2
1	B	215	VAL	2.2
1	D	9	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	218	ARG	2.2
1	C	365	GLY	2.2
1	D	411	ASP	2.2
1	A	95	ILE	2.2
1	D	392	LEU	2.2
1	A	78	TYR	2.1
1	B	266	ALA	2.1
1	D	319	GLN	2.1
1	D	418	ILE	2.1
1	B	214	VAL	2.1
1	A	246	ARG	2.1
1	A	326	GLU	2.1
1	C	86	GLU	2.1
1	A	71	HIS	2.1
1	B	418	ILE	2.1
1	D	25	THR	2.0
1	C	421	LYS	2.0
1	D	488	TYR	2.0
1	B	394	ILE	2.0
1	A	393	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	SO4	D	507	5/5	0.89	0.36	4.67	27,27,28,41	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAP	A	506	31/48	0.88	0.29	3.28	41,42,44,48	31
2	NAP	D	506	31/48	0.87	0.33	2.41	36,37,39,40	31
2	NAP	C	506	31/48	0.90	0.24	1.91	42,43,47,48	31
2	NAP	B	506	31/48	0.92	0.20	1.11	41,41,42,44	31
3	SO4	A	507	5/5	0.98	0.14	0.34	37,37,37,44	5
3	SO4	C	507	5/5	0.95	0.15	-0.14	30,36,37,38	5
3	SO4	B	507	5/5	0.94	0.13	-0.80	42,42,42,43	5

6.5 Other polymers

There are no such residues in this entry.