



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:23 PM GMT

PDB ID : 2CDC  
Title : SULFOLOBUS SOLFATARICUS GLUCOSE DEHYDROGENASE 1 IN  
COMPLEX WITH NADP AND XYLOSE  
Authors : Milburn, C.C.; Lamble, H.J.; Theodossis, A.; Hough, D.W.; Danson, M.J.;  
Taylor, G.L.  
Deposited on : 2006-01-23  
Resolution : 1.50 Å(reported)

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

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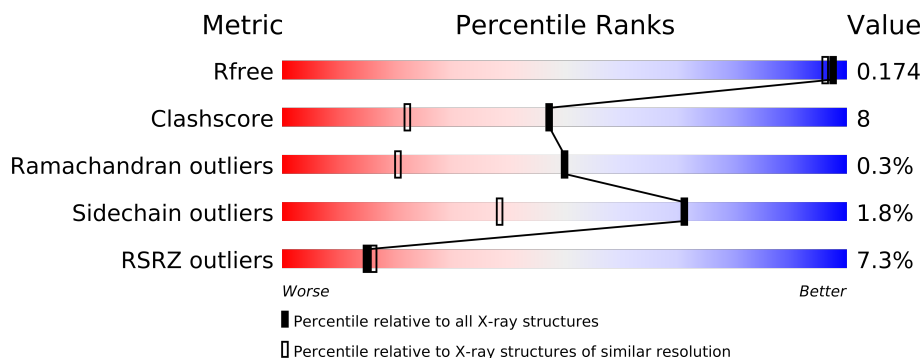
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	366	
1	B	366	
1	C	366	
1	D	366	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	XYS	A	1370	-	X
4	XYP	C	1369	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13649 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 GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	34	0
			2969	1902	501	552	14			
1	B	359	Total	C	N	O	S	0	26	0
			2937	1881	497	546	13			
1	C	359	Total	C	N	O	S	0	22	0
			2929	1875	497	543	14			
1	D	359	Total	C	N	O	S	0	22	0
			2922	1868	496	543	15			

There are 4 discrepancies between the modelled and reference sequences:

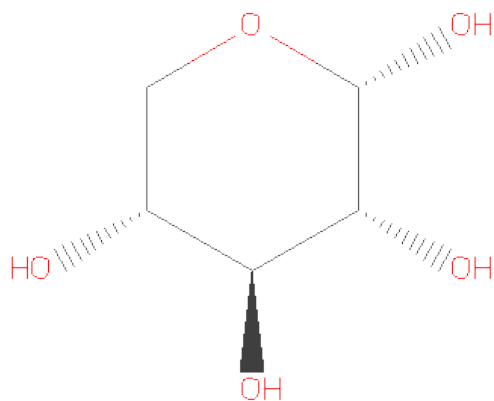
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	THR	ENGINEERED MUTATION	UNP O93715
B	41	ALA	THR	ENGINEERED MUTATION	UNP O93715
C	41	ALA	THR	ENGINEERED MUTATION	UNP O93715
D	41	ALA	THR	ENGINEERED MUTATION	UNP O93715

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



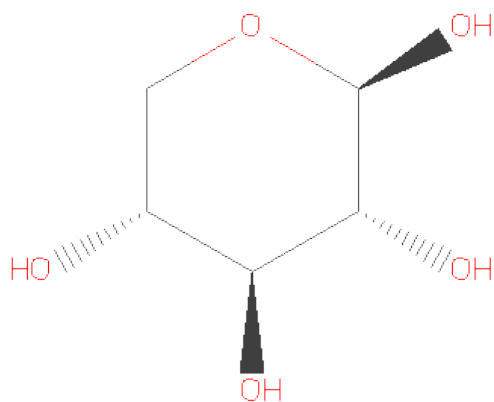
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is SUGAR (XYLOPYRANOSE) (three-letter code: XYS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	1
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula:  $C_5H_{10}O_5$ ).

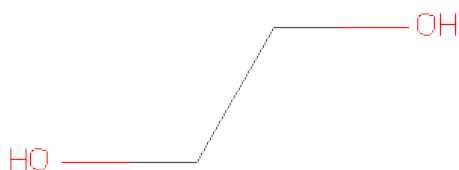


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		
4	D	1	Total	C	O	0	1
			10	5	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	A	2	Total 2	Zn 2	0	0
5	D	2	Total 2	Zn 2	0	0
5	C	2	Total 2	Zn 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	376	Total 376	O 376	0	0
7	B	401	Total 401	O 401	0	0
7	C	411	Total 411	O 411	0	0

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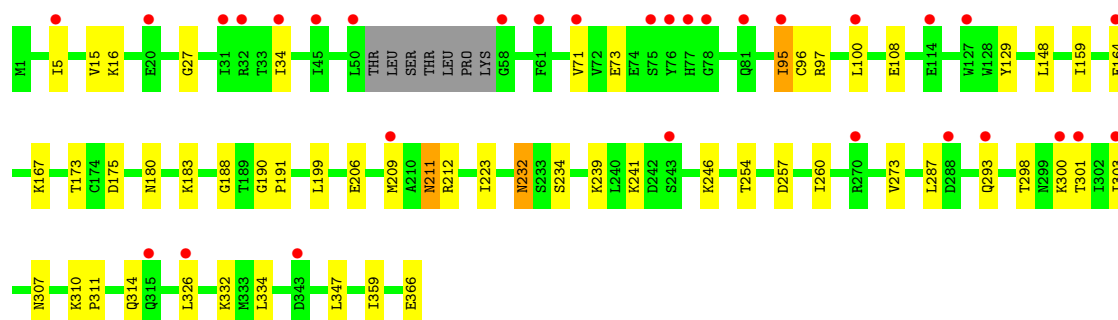
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	392	Total 392	O 392	0	0

### 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.

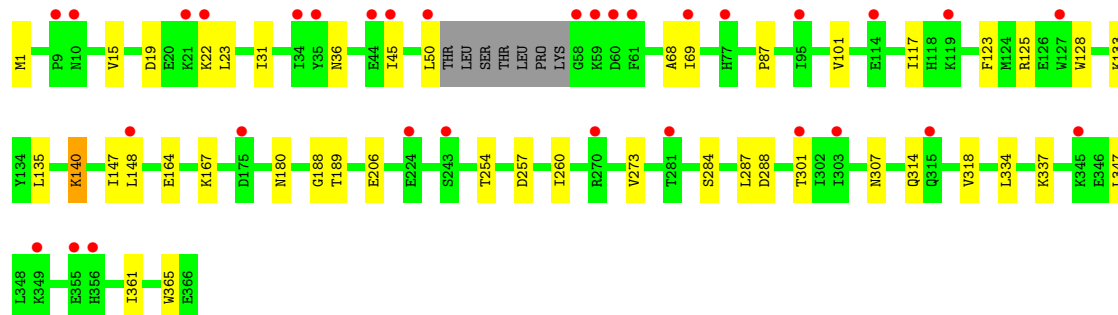
- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain A: 



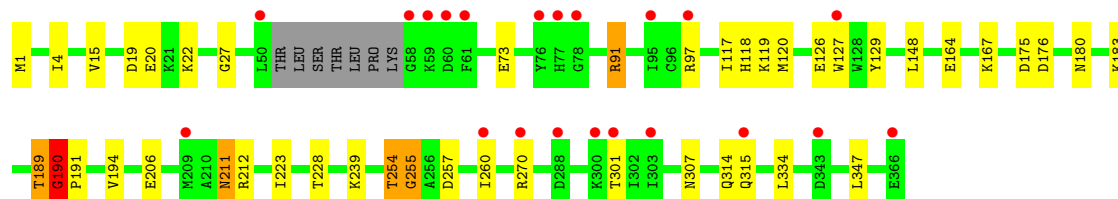
- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain B: 



- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

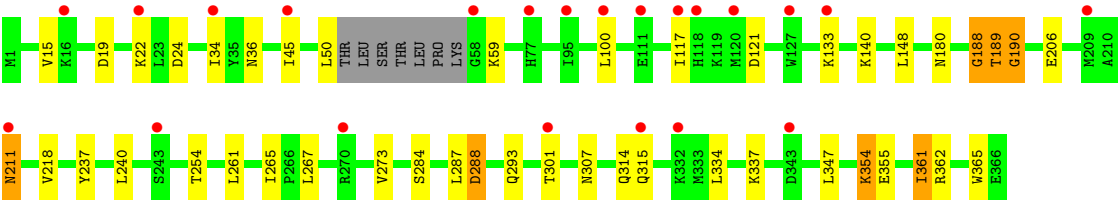
Chain C: 



- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.64Å 91.03Å 138.72Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	138.68 – 1.50 41.23 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (138.68-1.50) 92.9 (41.23-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.204 , 0.239 0.161 , 0.174	Depositor DCC
$R_{free}$ test set	12721 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.9	EDS
Estimated twinning fraction	0.279 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 253226 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.4868e-03.*

<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: XYP, ZN, XYS, EDO, NAP

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	0.59	2/3145 (0.1%)	0.80	4/4250 (0.1%)
1	B	0.46	0/3072	0.61	0/4147
1	C	0.84	8/3047 (0.3%)	0.73	12/4118 (0.3%)
1	D	1.27	6/3038 (0.2%)	0.84	12/4104 (0.3%)
All	All	0.85	16/12302 (0.1%)	0.75	28/16619 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	1	0
All	All	1	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189[A]	THR	N-CA	30.69	2.07	1.46
1	D	189[B]	THR	N-CA	30.69	2.07	1.46
1	D	190[A]	GLY	N-CA	28.02	1.88	1.46
1	D	190[B]	GLY	N-CA	28.02	1.88	1.46
1	D	189[A]	THR	CA-CB	20.06	2.05	1.53
1	D	189[B]	THR	CA-CB	20.06	2.05	1.53
1	C	190[A]	GLY	C-N	17.43	1.67	1.34
1	C	190[B]	GLY	C-N	17.43	1.67	1.34
1	C	255[A]	GLY	N-CA	14.85	1.68	1.46
1	C	255[B]	GLY	N-CA	14.85	1.68	1.46
1	A	95[A]	ILE	CG1-CD1	13.55	2.44	1.50
1	A	95[B]	ILE	CG1-CD1	13.55	2.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189[A]	THR	CA-C	11.68	1.83	1.52
1	C	189[B]	THR	CA-C	11.68	1.83	1.52
1	C	254[A]	THR	CA-C	7.79	1.73	1.52
1	C	254[B]	THR	CA-C	7.79	1.73	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95[A]	ILE	CG1-CB-CG2	-20.44	66.43	111.40
1	A	95[B]	ILE	CG1-CB-CG2	-20.44	66.43	111.40
1	D	189[A]	THR	N-CA-CB	-17.91	76.27	110.30
1	D	189[B]	THR	N-CA-CB	-17.91	76.27	110.30
1	A	95[A]	ILE	CB-CG1-CD1	-12.60	78.63	113.90
1	A	95[B]	ILE	CB-CG1-CD1	-12.60	78.63	113.90
1	D	189[A]	THR	CB-CA-C	-10.91	82.14	111.60
1	D	189[B]	THR	CB-CA-C	-10.91	82.14	111.60
1	D	189[A]	THR	CA-CB-OG1	10.87	131.82	109.00
1	D	189[B]	THR	CA-CB-OG1	10.87	131.82	109.00
1	C	254[A]	THR	CA-C-N	-8.12	99.97	116.20
1	C	254[B]	THR	CA-C-N	-8.12	99.97	116.20
1	D	189[A]	THR	C-N-CA	-7.75	106.01	122.30
1	D	189[B]	THR	C-N-CA	-7.75	106.01	122.30
1	D	188[A]	GLY	C-N-CA	-7.04	104.10	121.70
1	D	188[B]	GLY	C-N-CA	-7.04	104.10	121.70
1	C	254[A]	THR	N-CA-C	6.74	129.20	111.00
1	C	254[B]	THR	N-CA-C	6.74	129.20	111.00
1	C	254[A]	THR	CA-C-O	6.60	133.96	120.10
1	C	254[B]	THR	CA-C-O	6.60	133.96	120.10
1	C	189[A]	THR	CB-CA-C	-6.14	95.03	111.60
1	C	189[B]	THR	CB-CA-C	-6.14	95.03	111.60
1	D	189[A]	THR	CA-CB-CG2	-5.53	104.66	112.40
1	D	189[B]	THR	CA-CB-CG2	-5.53	104.66	112.40
1	C	190[A]	GLY	O-C-N	-5.42	110.81	121.10
1	C	190[B]	GLY	O-C-N	-5.42	110.81	121.10
1	C	254[A]	THR	C-N-CA	-5.05	111.68	122.30
1	C	254[B]	THR	C-N-CA	-5.05	111.68	122.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	189[B]	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	190[B]	GLY	Mainchain

## 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	A	2969	0	3029	52	0
1	B	2937	0	3007	47	0
1	C	2929	0	2981	55	0
1	D	2922	0	2972	52	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	3	0
3	A	20	0	20	1	0
3	B	10	0	10	0	0
3	C	10	0	10	0	0
3	D	20	0	20	0	0
4	A	10	0	10	1	0
4	B	10	0	10	0	0
4	C	10	0	10	0	0
4	D	10	0	10	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
6	D	4	0	6	1	0
7	A	376	0	0	9	0
7	B	401	0	0	14	0
7	C	411	0	0	7	0
7	D	392	0	0	12	0
All	All	13649	0	12207	194	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (194) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:CG2	1.26	1.58
1:C:254[B]:THR:C	1:C:254[B]:THR:CA	1.75	1.52
1:C:255[A]:GLY:N	1:C:255[A]:GLY:CA	1.68	1.51
1:C:189[A]:THR:C	1:C:189[A]:THR:CA	1.83	1.45
1:D:190[A]:GLY:CA	1:D:190[A]:GLY:N	1.88	1.36
1:D:189[A]:THR:CA	1:D:189[A]:THR:CB	2.05	1.34
1:A:34[B]:ILE:CD1	1:A:71[B]:VAL:CG2	2.16	1.22
1:D:189[A]:THR:CA	1:D:189[A]:THR:N	2.07	1.17
1:D:267:LEU:HD21	7:D:2256:HOH:O	1.45	1.13
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:HG21	1.28	1.08
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:HG23	1.29	1.07
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:HG22	1.37	1.02
1:B:189[A]:THR:O	7:B:2232:HOH:O	1.78	1.01
1:C:254[B]:THR:O	7:C:2294:HOH:O	1.79	1.00
1:C:117:ILE:HD12	7:C:2152:HOH:O	1.63	0.98
1:C:254[B]:THR:CB	1:C:254[B]:THR:C	2.32	0.97
1:C:254[B]:THR:C	1:C:254[B]:THR:N	2.18	0.97
1:A:95[A]:ILE:CG1	1:A:95[A]:ILE:CD1	2.44	0.94
1:A:180:ASN:HD21	1:B:314:GLN:HE22	1.17	0.93
1:D:254[A]:THR:O	7:D:2279:HOH:O	1.86	0.92
1:A:148:LEU:HD11	1:A:334:LEU:HB3	1.51	0.92
1:A:211:ASN:HD22	1:A:212:ARG:H	1.18	0.91
1:D:189[A]:THR:CB	1:D:189[A]:THR:C	2.37	0.91
1:A:34[B]:ILE:CD1	1:A:71[B]:VAL:HG23	1.91	0.90
1:C:211:ASN:HD22	1:C:212:ARG:H	1.17	0.89
1:C:254[B]:THR:C	1:C:254[B]:THR:OG1	2.12	0.88
1:A:314:GLN:HE22	1:B:180:ASN:HD21	1.15	0.87
1:A:183:LYS:HE3	7:A:2240:HOH:O	1.73	0.87
1:C:190[B]:GLY:O	1:C:191[B]:PRO:C	2.05	0.86
1:C:314:GLN:HE22	1:D:180:ASN:HD21	1.18	0.85
1:B:45:ILE:HD11	1:B:117:ILE:HG13	1.57	0.85
1:C:148:LEU:HD11	1:C:334:LEU:HB3	1.59	0.83
1:D:240:LEU:HB3	7:D:2256:HOH:O	1.80	0.82
1:D:45[A]:ILE:HD11	1:D:117:ILE:HG13	1.61	0.81
1:C:180:ASN:HD21	1:D:314:GLN:HE22	1.30	0.80
1:C:254[A]:THR:C	1:C:255[A]:GLY:CA	2.50	0.80
1:C:189[A]:THR:C	1:C:189[A]:THR:CB	2.51	0.79
1:A:34[B]:ILE:CD1	1:A:71[B]:VAL:HG22	2.02	0.79
1:A:254[A]:THR:O	7:A:2251:HOH:O	2.01	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:254[B]:THR:CA	1:C:255[B]:GLY:N	2.45	0.79
1:D:211[A]:ASN:HD21	2:D:1368:NAP:H1B	1.47	0.79
1:A:95[A]:ILE:CD1	1:A:95[A]:ILE:CB	2.61	0.78
1:D:148:LEU:HD11	1:D:334:LEU:HB3	1.65	0.77
1:B:128:TRP:CH2	7:B:2107:HOH:O	2.38	0.77
1:B:254[A]:THR:O	7:B:2296:HOH:O	2.02	0.77
1:C:183:LYS:HE3	7:C:2286:HOH:O	1.86	0.76
1:C:176:ASP:HB3	1:D:133[B]:LYS:HD2	1.67	0.76
1:D:45[A]:ILE:HG12	1:D:50:LEU:HD12	1.68	0.75
1:A:97:ARG:NH1	1:C:175:ASP:OD1	2.22	0.73
1:A:175:ASP:OD1	1:C:97[B]:ARG:NH1	2.22	0.73
1:B:1:MET:HE2	1:B:23:LEU:CD1	2.20	0.72
1:A:211:ASN:HD22	1:A:212:ARG:N	1.89	0.71
1:D:189[A]:THR:C	1:D:190[A]:GLY:CA	2.59	0.70
1:C:211:ASN:HD22	1:C:212:ARG:N	1.90	0.70
1:D:100[A]:LEU:HD23	7:D:2038:HOH:O	1.92	0.70
1:B:1:MET:CE	1:B:23:LEU:CD1	2.70	0.69
1:A:326[A]:LEU:HD13	7:B:2400:HOH:O	1.92	0.69
1:D:189[A]:THR:CB	1:D:189[A]:THR:N	2.55	0.69
1:D:189[A]:THR:HB	1:D:189[A]:THR:O	1.92	0.69
1:A:15:VAL:HG21	1:A:347:LEU:HD23	1.74	0.68
1:D:189[A]:THR:HB	1:D:189[A]:THR:C	2.15	0.67
1:D:189[A]:THR:HG1	2:D:1368:NAP:HO3A	1.43	0.67
1:D:237:TYR:HB3	7:D:2256:HOH:O	1.94	0.66
1:A:96:CYS:O	1:A:100[B]:LEU:HD13	1.97	0.65
1:C:270[B]:ARG:NH1	7:C:2308:HOH:O	2.30	0.64
1:B:140:LYS:HG3	7:B:2193:HOH:O	1.98	0.64
1:C:4:ILE:HG12	1:C:15:VAL:HG22	1.80	0.64
1:C:164:GLU:HA	1:C:167:LYS:HE2	1.80	0.64
1:B:19:ASP:HB3	1:B:22:LYS:HE2	1.79	0.63
1:C:148:LEU:CD1	1:C:334:LEU:HB3	2.29	0.63
1:A:100[A]:LEU:HD23	7:A:2037:HOH:O	1.98	0.63
1:B:1:MET:HE2	1:B:23:LEU:HD11	1.81	0.63
1:D:337:LYS:HG2	1:D:361:ILE:HD13	1.80	0.62
1:D:354:LYS:NZ	1:D:354:LYS:HB2	2.14	0.62
1:A:188[A]:GLY:HA3	1:A:254[A]:THR:HG22	1.82	0.61
1:A:148:LEU:CD1	1:A:334:LEU:HB3	2.28	0.60
1:A:173:THR:O	1:C:97[A]:ARG:NH1	2.26	0.59
1:D:36:ASN:ND2	1:D:365:TRP:HE1	2.00	0.59
1:A:209[A]:MET:CE	1:A:223:ILE:HG13	2.33	0.59
1:A:34[B]:ILE:CG1	1:A:71[B]:VAL:HG23	2.31	0.58
1:D:45[A]:ILE:CD1	1:D:117:ILE:HG13	2.34	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:ALA:HB3	7:B:2107:HOH:O	2.03	0.58
1:A:366:GLU:HB2	7:A:2320:HOH:O	2.04	0.58
1:C:189[A]:THR:CA	1:C:190[A]:GLY:N	2.60	0.58
1:D:188[A]:GLY:C	1:D:189[A]:THR:CA	2.72	0.58
1:C:118:HIS:NE2	1:C:119:LYS:HE2	2.19	0.58
1:B:68:ALA:CB	7:B:2107:HOH:O	2.52	0.57
1:A:303[B]:ILE:HG12	1:C:301[B]:THR:HG22	1.85	0.57
1:A:95[B]:ILE:CG2	1:A:95[B]:ILE:CG1	2.82	0.57
1:A:232:ASN:C	1:A:232:ASN:HD22	2.09	0.56
1:D:148:LEU:HD13	1:D:334:LEU:HD13	1.87	0.56
3:A:1368[A]:XYS:H52	7:A:2358:HOH:O	2.06	0.56
4:A:1369[B]:XYP:H5B2	7:A:2358:HOH:O	2.06	0.56
1:B:1:MET:HE1	1:B:23:LEU:HD13	1.88	0.56
1:B:148[A]:LEU:HD11	1:B:334:LEU:HB3	1.88	0.56
1:B:36:ASN:ND2	1:B:365:TRP:HE1	2.05	0.55
1:B:148[A]:LEU:HD13	1:B:334:LEU:HD13	1.89	0.54
1:A:298:THR:CB	1:A:300[B]:LYS:HZ3	2.21	0.54
1:D:45[A]:ILE:CG1	1:D:50:LEU:HD12	2.38	0.54
1:B:87:PRO:HG3	7:B:2107:HOH:O	2.07	0.54
1:B:123:PHE:HB3	7:B:2107:HOH:O	2.07	0.54
1:C:148:LEU:HD13	1:C:334:LEU:HD13	1.89	0.53
1:C:15:VAL:HG21	1:C:347:LEU:HD23	1.89	0.53
1:D:36:ASN:HD22	1:D:365:TRP:HE1	1.54	0.53
2:D:1368:NAP:H2A	7:D:2253:HOH:O	2.09	0.53
1:B:1:MET:HE1	1:B:23:LEU:CD1	2.38	0.53
1:A:164[A]:GLU:HA	1:A:167:LYS:HE2	1.90	0.53
1:A:206:GLU:HG2	7:A:2187:HOH:O	2.09	0.53
1:C:257:ASP:O	1:C:260[A]:ILE:HG22	2.08	0.52
1:A:95[B]:ILE:CD1	1:A:95[B]:ILE:CG1	2.88	0.52
1:C:189[B]:THR:O	2:C:1368:NAP:H4B	2.09	0.52
1:D:148:LEU:CD1	1:D:334:LEU:HB3	2.39	0.52
1:A:273:VAL:HG22	1:A:301[B]:THR:CG2	2.39	0.52
1:B:45:ILE:HG12	1:B:50:LEU:HD12	1.91	0.52
1:B:206:GLU:HG2	7:B:2235:HOH:O	2.10	0.51
1:D:189[A]:THR:CA	1:D:189[A]:THR:CG2	2.87	0.51
1:C:1:MET:HG2	1:C:126:GLU:HB2	1.92	0.51
1:D:273:VAL:HG22	1:D:301[B]:THR:CG2	2.41	0.50
1:C:254[B]:THR:C	1:C:254[B]:THR:H	2.09	0.50
1:A:232:ASN:HD22	1:A:234:SER:H	1.60	0.50
1:D:261:LEU:O	1:D:265:ILE:HG13	2.12	0.50
1:B:288:ASP:HA	1:D:284:SER:HA	1.93	0.49
1:A:159:ILE:HD12	1:A:199:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:ASP:O	1:A:260:ILE:HG22	2.12	0.49
1:B:337:LYS:HG2	1:B:361:ILE:HD12	1.95	0.49
1:C:1:MET:CG	1:C:126:GLU:HB2	2.43	0.49
1:A:190[A]:GLY:HA2	7:A:2204:HOH:O	2.12	0.49
1:B:284:SER:HA	1:D:288:ASP:HA	1.94	0.49
1:B:45:ILE:CD1	1:B:117:ILE:HG13	2.35	0.49
1:C:118:HIS:CD2	1:C:119:LYS:HE2	2.48	0.48
1:C:1:MET:HE2	1:C:20:GLU:HG2	1.94	0.48
1:C:211:ASN:ND2	1:C:212:ARG:H	1.99	0.48
1:D:315[A]:GLN:NE2	7:D:2321:HOH:O	2.45	0.48
1:B:337:LYS:HG2	1:B:361:ILE:CD1	2.44	0.48
1:A:95[A]:ILE:CD1	1:A:95[A]:ILE:HB	2.42	0.47
1:B:318:VAL:HG22	7:B:2400:HOH:O	2.13	0.47
1:B:188[A]:GLY:HA3	1:B:254[A]:THR:HG22	1.97	0.47
1:C:206:GLU:HG2	7:C:2224:HOH:O	2.14	0.47
1:C:127[A]:TRP:HZ3	1:C:129:TYR:CE2	2.33	0.47
1:C:27:GLY:O	1:C:129:TYR:HB3	2.14	0.47
1:A:332:LYS:HG3	7:A:2307:HOH:O	2.13	0.47
1:D:24:ASP:HB2	1:D:121:ASP:HB2	1.97	0.47
1:A:232:ASN:ND2	1:A:234:SER:H	2.13	0.47
1:B:36:ASN:HD22	1:B:365:TRP:HE1	1.62	0.47
1:B:15:VAL:HG21	1:B:347:LEU:HD23	1.97	0.46
1:B:257:ASP:O	1:B:260:ILE:HG22	2.16	0.46
1:A:191[A]:PRO:HD3	1:A:359:ILE:HA	1.96	0.46
1:D:354:LYS:HB2	1:D:354:LYS:HZ2	1.81	0.46
1:C:257:ASP:O	1:C:260[B]:ILE:HG23	2.15	0.46
1:A:27:GLY:O	1:A:129:TYR:HB3	2.16	0.46
1:A:180:ASN:ND2	1:B:314:GLN:HE22	1.99	0.46
1:A:310:LYS:N	1:A:311:PRO:HD2	2.32	0.45
1:C:190[B]:GLY:H	1:C:194:VAL:HG23	1.82	0.45
1:B:1:MET:CE	1:B:125:ARG:HB2	2.46	0.45
1:D:189[B]:THR:O	1:D:190[B]:GLY:O	2.35	0.45
1:A:108:GLU:C	1:C:270[B]:ARG:HE	2.20	0.44
1:C:315[B]:GLN:HG3	7:C:2339:HOH:O	2.17	0.44
1:B:101:VAL:HA	1:C:97[A]:ARG:HE	1.81	0.44
1:D:206:GLU:HG2	7:D:2218:HOH:O	2.18	0.44
1:D:354:LYS:HB2	1:D:354:LYS:HZ3	1.82	0.44
1:D:133[B]:LYS:HG2	7:D:2049:HOH:O	2.18	0.44
1:B:273:VAL:HG22	1:B:301[B]:THR:CG2	2.48	0.43
1:B:69[A]:ILE:HD11	1:B:147:ILE:N	2.34	0.43
1:B:117:ILE:HD13	7:B:2163:HOH:O	2.18	0.43
1:B:148[A]:LEU:CD1	1:B:334:LEU:HB3	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:128:TRP:CZ2	7:B:2107:HOH:O	2.69	0.42
1:C:1:MET:HB2	1:C:20:GLU:HG3	2.01	0.42
1:A:100[B]:LEU:HD23	1:D:100[B]:LEU:HD11	2.01	0.42
1:D:189[A]:THR:O	1:D:190[A]:GLY:CA	2.68	0.42
1:C:189[A]:THR:C	1:C:189[A]:THR:HB	2.37	0.42
1:A:209[A]:MET:HE3	1:A:223:ILE:HG13	2.02	0.42
1:A:5[A]:ILE:HD11	1:A:16:LYS:HD3	2.02	0.42
1:B:337:LYS:CG	1:B:361:ILE:HD12	2.50	0.42
1:C:1:MET:CE	1:C:20:GLU:HG2	2.49	0.42
1:D:354:LYS:CB	1:D:354:LYS:NZ	2.80	0.41
1:D:355:GLU:HG3	7:D:2368:HOH:O	2.19	0.41
1:D:19:ASP:HB3	1:D:22:LYS:HE2	2.03	0.41
1:B:45:ILE:CG1	1:B:50:LEU:HD12	2.50	0.41
1:D:140:LYS:HD2	6:D:1367:EDO:O1	2.20	0.41
1:C:255[B]:GLY:HA2	7:C:2294:HOH:O	2.21	0.41
1:D:315[A]:GLN:NE2	7:D:2322:HOH:O	2.53	0.41
1:D:218:VAL:HG23	7:D:2231:HOH:O	2.20	0.41
1:B:164:GLU:HG3	7:B:2207:HOH:O	2.19	0.41
1:B:164:GLU:HA	1:B:167:LYS:HE3	2.02	0.41
1:A:241:LYS:HE3	1:A:246:LYS:HE2	2.02	0.41
1:C:223:ILE:HG23	1:C:228:THR:O	2.20	0.41
1:B:31:ILE:HD11	1:B:135:LEU:HD11	2.02	0.41
1:C:19:ASP:HB3	1:C:22:LYS:NZ	2.36	0.41
1:B:1:MET:HE3	1:B:125:ARG:HB2	2.03	0.40
1:C:254[B]:THR:O	1:C:254[B]:THR:OG1	2.38	0.40
1:C:91:ARG:HG3	1:C:120:MET:SD	2.62	0.40
1:D:15:VAL:HG21	1:D:347:LEU:HD23	2.04	0.40
1:D:190[A]:GLY:C	1:D:190[A]:GLY:N	2.69	0.40
1:B:1:MET:CE	1:B:23:LEU:HD13	2.46	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/366 (106%)	380 (98%)	8 (2%)	1 (0%)	50	20
1	B	381/366 (104%)	371 (97%)	9 (2%)	1 (0%)	50	20
1	C	377/366 (103%)	364 (97%)	12 (3%)	1 (0%)	50	20
1	D	377/366 (103%)	368 (98%)	8 (2%)	1 (0%)	50	20
All	All	1524/1464 (104%)	1483 (97%)	37 (2%)	4 (0%)	50	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	307	ASN
1	C	307	ASN
1	D	307	ASN

### 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	339/317 (107%)	332 (98%)	7 (2%)	66	30
1	B	331/317 (104%)	328 (99%)	3 (1%)	87	69
1	C	327/317 (103%)	323 (99%)	4 (1%)	82	57
1	D	327/317 (103%)	317 (97%)	10 (3%)	52	15
All	All	1324/1268 (104%)	1300 (98%)	24 (2%)	71	38

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	211	ASN
1	A	232	ASN
1	A	239	LYS
1	A	287	LEU
1	A	293[A]	GLN
1	A	293[B]	GLN
1	B	133	LYS

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Mol	Chain	Res	Type
1	B	140	LYS
1	B	287	LEU
1	C	73	GLU
1	C	91	ARG
1	C	211	ASN
1	C	239	LYS
1	D	34	ILE
1	D	59	LYS
1	D	211[A]	ASN
1	D	211[B]	ASN
1	D	287	LEU
1	D	288	ASP
1	D	293	GLN
1	D	354	LYS
1	D	361	ILE
1	D	362	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	211	ASN
1	A	232	ASN
1	A	259	ASN
1	A	297	HIS
1	A	314	GLN
1	B	36	ASN
1	B	118	HIS
1	B	259	ASN
1	B	293	GLN
1	B	297	HIS
1	B	314	GLN
1	C	47	ASN
1	C	211	ASN
1	C	259	ASN
1	C	297	HIS
1	C	314	GLN
1	D	36	ASN
1	D	77	HIS
1	D	259	ASN
1	D	314	GLN

### 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 ⓘ

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAP	A	1367	-	52,52,52	1.30	6 (11%)	80,80,80	1.77	11 (13%)
3	XYS	A	1368[A]	-	10,10,10	1.09	1 (10%)	14,14,14	1.05	0
4	XYP	A	1369[B]	-	10,10,10	1.14	1 (10%)	14,14,14	1.06	0
3	XYS	A	1370	-	10,10,10	0.81	0	14,14,14	1.23	1 (7%)
6	EDO	B	1367	-	3,3,3	0.71	0	2,2,2	0.18	0
2	NAP	B	1368	-	52,52,52	1.17	4 (7%)	80,80,80	1.77	13 (16%)
4	XYP	B	1369	-	10,10,10	1.11	2 (20%)	14,14,14	0.74	0
3	XYS	B	1370	-	10,10,10	1.19	1 (10%)	14,14,14	1.00	1 (7%)
6	EDO	C	1367	-	3,3,3	0.68	0	2,2,2	0.13	0
2	NAP	C	1368	-	52,52,52	1.23	5 (9%)	80,80,80	1.57	9 (11%)
4	XYP	C	1369	-	10,10,10	1.05	0	14,14,14	0.69	0
3	XYS	C	1370	-	10,10,10	1.11	1 (10%)	14,14,14	1.10	1 (7%)
6	EDO	D	1367	-	3,3,3	0.72	0	2,2,2	0.03	0
2	NAP	D	1368	-	52,52,52	1.30	6 (11%)	80,80,80	1.73	14 (17%)
3	XYS	D	1369[A]	-	10,10,10	1.11	1 (10%)	14,14,14	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	XYP	D	1370[B]	-	10,10,10	1.13	1 (10%)	14,14,14	0.83	0
3	XYS	D	1371	-	10,10,10	0.95	1 (10%)	14,14,14	0.93	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	1367	-	-	0/35/67/67	0/3/5/5
3	XYS	A	1368[A]	-	-	0/0/17/17	0/1/1/1
4	XYP	A	1369[B]	-	-	0/0/17/17	0/1/1/1
3	XYS	A	1370	-	-	0/0/17/17	0/1/1/1
6	EDO	B	1367	-	-	0/1/1/1	0/0/0/0
2	NAP	B	1368	-	-	0/35/67/67	0/3/5/5
4	XYP	B	1369	-	-	0/0/17/17	0/1/1/1
3	XYS	B	1370	-	-	0/0/17/17	0/1/1/1
6	EDO	C	1367	-	-	0/1/1/1	0/0/0/0
2	NAP	C	1368	-	-	0/35/67/67	0/3/5/5
4	XYP	C	1369	-	-	0/0/17/17	0/1/1/1
3	XYS	C	1370	-	-	0/0/17/17	0/1/1/1
6	EDO	D	1367	-	-	0/1/1/1	0/0/0/0
2	NAP	D	1368	-	-	0/35/67/67	0/3/5/5
3	XYS	D	1369[A]	-	-	0/0/17/17	0/1/1/1
4	XYP	D	1370[B]	-	-	0/0/17/17	0/1/1/1
3	XYS	D	1371	-	-	0/0/17/17	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1367	NAP	C2N-N1N	4.16	1.40	1.35
2	D	1368	NAP	C2N-N1N	4.14	1.40	1.35
2	B	1368	NAP	C2N-N1N	4.05	1.40	1.35
2	C	1368	NAP	C2N-N1N	3.85	1.40	1.35
2	C	1368	NAP	P2B-O1X	3.72	1.63	1.51
2	D	1368	NAP	C4A-N9A	-3.63	1.32	1.37
2	B	1368	NAP	P2B-O1X	3.41	1.62	1.51
2	D	1368	NAP	O4D-C1D	3.34	1.46	1.41
2	A	1367	NAP	C4A-N9A	-3.24	1.33	1.37
2	A	1367	NAP	PN-O3	3.12	1.66	1.60
2	A	1367	NAP	O4B-C1B	2.99	1.45	1.41
3	D	1369[A]	XYS	O5-C5	2.89	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1370[B]	XYP	O5B-C5B	2.89	1.48	1.43
2	C	1368	NAP	C4A-N9A	-2.86	1.33	1.37
2	D	1368	NAP	P2B-O1X	2.84	1.60	1.51
2	C	1368	NAP	O4D-C1D	2.80	1.45	1.41
3	C	1370	XYS	O5-C1	2.80	1.47	1.43
2	B	1368	NAP	C4A-N9A	-2.65	1.33	1.37
2	A	1367	NAP	P2B-O1X	2.65	1.60	1.51
3	D	1371	XYS	O5-C1	2.52	1.46	1.43
2	C	1368	NAP	P2B-O2X	2.41	1.63	1.54
4	A	1369[B]	XYP	O5B-C5B	2.41	1.47	1.43
3	A	1368[A]	XYS	O5-C5	2.41	1.47	1.43
2	D	1368	NAP	O4B-C1B	2.41	1.45	1.41
3	B	1370	XYS	O5-C1	2.36	1.46	1.43
4	B	1369	XYP	O5B-C1B	2.32	1.46	1.43
2	B	1368	NAP	C6N-N1N	2.27	1.41	1.35
4	B	1369	XYP	O5B-C5B	2.20	1.47	1.43
2	A	1367	NAP	P2B-O2X	2.16	1.62	1.54
2	D	1368	NAP	PA-O3	2.04	1.63	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1367	NAP	N3A-C2A-N1A	-10.47	119.96	128.71
2	B	1368	NAP	N3A-C2A-N1A	-9.46	120.80	128.71
2	D	1368	NAP	N3A-C2A-N1A	-8.66	121.47	128.71
2	C	1368	NAP	N3A-C2A-N1A	-8.54	121.57	128.71
2	D	1368	NAP	O4D-C1D-N1N	-4.50	103.34	107.95
2	D	1368	NAP	N3A-C4A-N9A	4.11	132.86	125.43
2	B	1368	NAP	N3A-C4A-N9A	4.11	132.85	125.43
2	A	1367	NAP	O4B-C1B-C2B	-4.01	103.20	106.95
2	B	1368	NAP	O4D-C1D-C2D	-3.82	100.92	106.77
2	A	1367	NAP	N3A-C4A-N9A	3.74	132.19	125.43
2	B	1368	NAP	O4B-C1B-C2B	-3.69	103.50	106.95
2	C	1368	NAP	O4B-C1B-C2B	-3.65	103.53	106.95
2	C	1368	NAP	N3A-C4A-N9A	3.62	131.97	125.43
2	D	1368	NAP	C8A-N9A-C4A	3.47	109.55	106.90
3	C	1370	XYS	C5-O5-C1	3.29	118.93	112.86
2	A	1367	NAP	O4D-C1D-C2D	-3.24	101.80	106.77
3	A	1370	XYS	C5-O5-C1	3.21	118.79	112.86
2	B	1368	NAP	C4B-O4B-C1B	-3.10	106.38	109.75
2	C	1368	NAP	C4A-C5A-N7A	-2.96	106.99	109.52
2	D	1368	NAP	O4B-C1B-C2B	-2.88	104.26	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1368	NAP	C3N-C7N-N7N	-2.85	114.53	117.77
2	B	1368	NAP	C2D-C1D-N1N	2.84	118.67	113.86
2	D	1368	NAP	C1B-N9A-C4A	-2.75	121.88	126.64
2	C	1368	NAP	O4D-C1D-C2D	-2.67	102.68	106.77
2	C	1368	NAP	C5A-C4A-N3A	-2.66	119.90	125.70
2	D	1368	NAP	O4D-C1D-C2D	-2.60	102.78	106.77
2	D	1368	NAP	C4B-O4B-C1B	-2.59	106.93	109.75
2	B	1368	NAP	C5A-C4A-N3A	-2.54	120.17	125.70
2	B	1368	NAP	C3N-C7N-N7N	-2.50	114.92	117.77
2	C	1368	NAP	C4B-O4B-C1B	-2.41	107.13	109.75
2	A	1367	NAP	O3X-P2B-O2X	2.37	116.85	107.61
2	D	1368	NAP	C4D-O4D-C1D	-2.35	107.19	109.75
2	A	1367	NAP	C2A-N3A-C4A	2.35	120.70	114.01
2	D	1368	NAP	C5A-C4A-N3A	-2.34	120.61	125.70
2	A	1367	NAP	C8A-N9A-C4A	2.33	108.68	106.90
2	B	1368	NAP	O4D-C1D-N1N	-2.31	105.58	107.95
3	B	1370	XYX	O5-C1-C2	-2.29	105.95	109.24
2	B	1368	NAP	C2A-N3A-C4A	2.28	120.51	114.01
2	A	1367	NAP	C5A-C4A-N3A	-2.28	120.73	125.70
2	B	1368	NAP	C2N-C3N-C4N	2.26	120.87	118.31
2	D	1368	NAP	O3X-P2B-O2B	2.25	113.56	107.09
2	B	1368	NAP	C4A-C5A-N7A	-2.24	107.61	109.52
2	A	1367	NAP	C4A-C5A-N7A	-2.23	107.61	109.52
2	A	1367	NAP	C4B-O4B-C1B	-2.23	107.33	109.75
2	C	1368	NAP	C2A-N3A-C4A	2.18	120.22	114.01
2	D	1368	NAP	C4A-C5A-N7A	-2.09	107.73	109.52
2	C	1368	NAP	C3N-C7N-N7N	-2.08	115.41	117.77
2	D	1368	NAP	N7A-C8A-N9A	-2.07	108.50	114.36
2	A	1367	NAP	C2A-N1A-C6A	2.07	122.51	118.77
2	B	1368	NAP	C1B-N9A-C4A	-2.04	123.12	126.64

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	A	359/366 (98%)	0.43	31 (8%)	11 11	7, 13, 25, 33	27 (7%)
1	B	359/366 (98%)	0.34	32 (8%)	10 10	7, 14, 26, 34	19 (5%)
1	C	359/366 (98%)	0.24	21 (5%)	22 24	7, 13, 25, 35	15 (4%)
1	D	359/366 (98%)	0.28	22 (6%)	21 22	7, 14, 25, 33	14 (3%)
All	All	1436/1464 (98%)	0.32	106 (7%)	15 16	7, 14, 25, 35	75 (5%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	HIS	8.2
1	A	5[A]	ILE	7.4
1	D	100[A]	LEU	7.4
1	A	31[A]	ILE	7.2
1	C	77	HIS	7.1
1	A	76[A]	TYR	7.0
1	A	95[A]	ILE	6.9
1	C	260[A]	ILE	6.8
1	C	50	LEU	6.5
1	A	50	LEU	6.4
1	B	34[A]	ILE	6.3
1	C	58	GLY	6.2
1	A	34[A]	ILE	6.2
1	D	45[A]	ILE	6.1
1	A	100[A]	LEU	6.1
1	A	45[A]	ILE	5.8
1	D	58	GLY	5.6
1	C	303[A]	ILE	5.6
1	A	293[A]	GLN	5.5
1	C	95[A]	ILE	5.3
1	C	76	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	243[A]	SER	5.0
1	B	303[A]	ILE	4.9
1	A	326[A]	LEU	4.8
1	D	243[A]	SER	4.8
1	B	349[A]	LYS	4.6
1	D	133[A]	LYS	4.6
1	B	69[A]	ILE	4.6
1	A	303[A]	ILE	4.6
1	B	58	GLY	4.6
1	A	243[A]	SER	4.5
1	B	59[A]	LYS	4.5
1	A	20[A]	GLU	4.4
1	A	300[A]	LYS	4.3
1	B	60[A]	ASP	4.1
1	C	301[A]	THR	4.0
1	B	127	TRP	4.0
1	B	148[A]	LEU	3.9
1	C	300[A]	LYS	3.8
1	A	343[A]	ASP	3.8
1	C	127[A]	TRP	3.8
1	D	315[A]	GLN	3.8
1	A	315[A]	GLN	3.8
1	C	209[A]	MET	3.7
1	D	118[A]	HIS	3.7
1	A	209[A]	MET	3.7
1	C	78	GLY	3.7
1	B	301[A]	THR	3.6
1	A	301[A]	THR	3.5
1	B	315[A]	GLN	3.5
1	A	32[A]	ARG	3.5
1	A	58	GLY	3.4
1	D	209[A]	MET	3.4
1	A	71[A]	VAL	3.4
1	C	288[A]	ASP	3.4
1	B	45	ILE	3.3
1	B	44[A]	GLU	3.3
1	D	301[A]	THR	3.3
1	A	270[A]	ARG	3.3
1	D	77	HIS	3.2
1	A	61	PHE	3.2
1	B	345[A]	LYS	3.2
1	B	61	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	315[A]	GLN	3.1
1	B	270[A]	ARG	3.0
1	A	127	TRP	3.0
1	B	175[A]	ASP	3.0
1	B	114[A]	GLU	3.0
1	D	332	LYS	3.0
1	D	211[A]	ASN	3.0
1	D	343[A]	ASP	2.9
1	C	270[A]	ARG	2.8
1	B	77	HIS	2.8
1	C	97[A]	ARG	2.8
1	C	343[A]	ASP	2.8
1	D	95	ILE	2.7
1	A	78	GLY	2.7
1	C	61	PHE	2.7
1	B	356	HIS	2.6
1	B	95	ILE	2.6
1	A	288[A]	ASP	2.6
1	A	164[A]	GLU	2.6
1	D	127	TRP	2.6
1	D	34	ILE	2.5
1	D	111[A]	GLU	2.5
1	B	9	PRO	2.5
1	B	119[A]	LYS	2.5
1	A	81[A]	GLN	2.5
1	D	270[A]	ARG	2.5
1	D	22	LYS	2.4
1	C	59	LYS	2.4
1	A	75	SER	2.4
1	C	60[A]	ASP	2.3
1	D	117	ILE	2.3
1	D	120[A]	MET	2.3
1	B	224[A]	GLU	2.3
1	B	21	LYS	2.3
1	B	10	ASN	2.2
1	B	22	LYS	2.2
1	A	114[A]	GLU	2.1
1	B	281	THR	2.1
1	B	35	TYR	2.1
1	B	50	LEU	2.1
1	C	366	GLU	2.0
1	D	16	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	355	GLU	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
4	XYP	C	1369	10/10	0.14	4.71	16,19,20,22	0
3	XYS	A	1370	10/10	0.12	2.96	15,17,19,20	0
3	XYS	D	1369[A]	10/10	0.19	1.48	18,21,22,23	10
3	XYS	D	1371	10/10	0.10	1.23	12,15,17,18	0
4	XYP	D	1370[B]	10/10	0.17	1.17	18,21,22,23	10
3	XYS	B	1370	10/10	0.13	0.82	13,15,17,19	0
3	XYS	A	1368[A]	10/10	0.15	0.75	13,17,19,20	10
3	XYS	C	1370	10/10	0.09	0.58	16,19,20,23	0
4	XYP	A	1369[B]	10/10	0.14	0.54	13,17,19,20	10
4	XYP	B	1369	10/10	0.13	0.18	18,21,24,24	0
2	NAP	B	1368	48/48	0.10	-0.25	12,16,18,21	0
5	ZN	A	1372	1/1	0.07	-0.41	10,10,10,10	0
2	NAP	D	1368	48/48	0.09	-0.45	12,15,17,20	0
6	EDO	C	1367	4/4	0.07	-0.50	13,15,16,16	0
2	NAP	C	1368	48/48	0.08	-0.52	9,13,17,17	0
6	EDO	B	1367	4/4	0.07	-0.62	16,17,18,18	0
6	EDO	D	1367	4/4	0.07	-0.73	17,18,19,20	0
5	ZN	B	1372	1/1	0.06	-0.88	12,12,12,12	0
5	ZN	C	1372	1/1	0.06	-0.89	10,10,10,10	0
5	ZN	C	1371	1/1	0.06	-0.90	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	D	1373	1/1	0.06	-1.04	11,11,11,11	0
2	NAP	A	1367	48/48	0.06	-1.24	10,13,16,17	0
5	ZN	D	1372	1/1	0.06	-2.22	11,11,11,11	1
5	ZN	A	1371	1/1	0.05	-3.18	10,10,10,10	1
5	ZN	B	1371	1/1	0.04	-3.51	10,10,10,10	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.