



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:06 am GMT

PDB ID : 3AI2  
Title : The crystal structure of L-sorbose reductase from *Gluconobacter frateurii* complexed with NADPH  
Authors : Kubota, K.; Nagata, K.; Okai, M.; Miyazono, K.; Tanokura, M.  
Deposited on : 2010-05-07  
Resolution : 1.90 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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

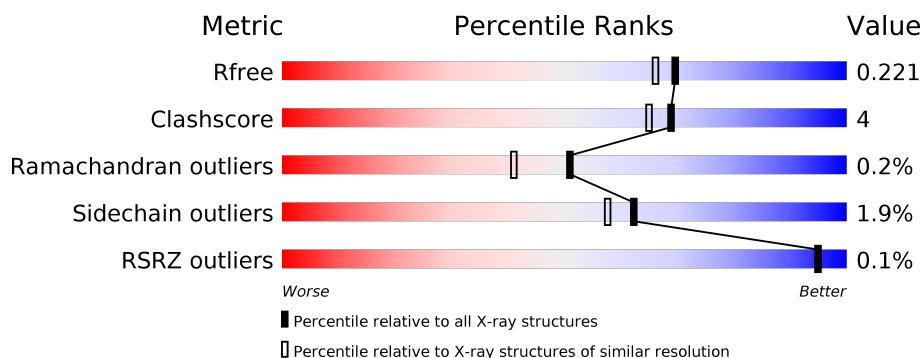
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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. 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	263	<div> <div>89%</div> <div>10% •</div> </div>
1	B	263	<div> <div>88%</div> <div>11% •</div> </div>
1	C	263	<div> <div>92%</div> <div>8%</div> </div>
1	D	263	<div> <div>92%</div> <div>8%</div> </div>
1	E	263	<div> <div>93%</div> <div>6%</div> </div>
1	F	263	<div> <div>90%</div> <div>8% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	263	<div><div></div><div>92%</div><div>8%</div></div>
1	H	263	<div><div></div><div>89%</div><div>9%</div></div>

## 2 Entry composition

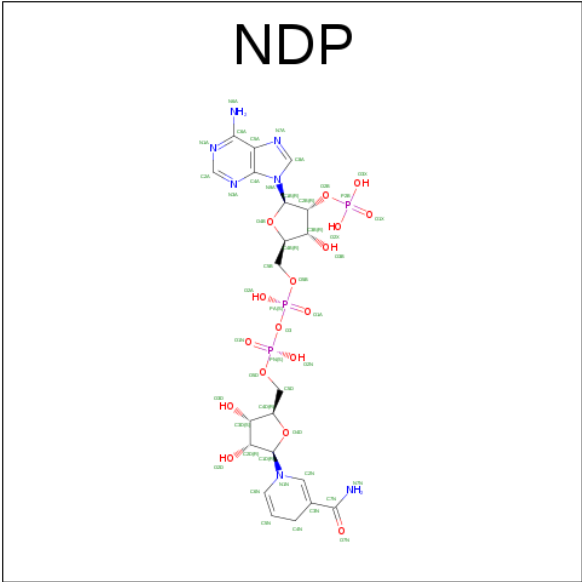
There are 3 unique types of molecules in this entry. The entry contains 17723 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADPH-sorbose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	B	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	H	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	D	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	E	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	C	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	F	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			
1	G	263	Total	C	N	O	S	0	0	0
			1991	1266	342	372	11			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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	H	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		
2	E	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	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	187	Total	O	0	0
			187	187		
3	H	201	Total	O	0	0
			201	201		
3	D	179	Total	O	0	0
			179	179		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	166	Total 166	O 166	0	0
3	C	169	Total 169	O 169	0	0
3	F	157	Total 157	O 157	0	0
3	G	169	Total 169	O 169	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

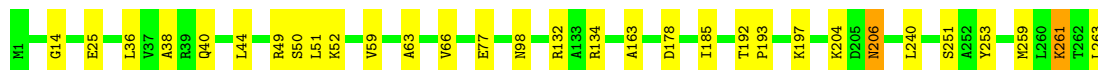
- Molecule 1: NADPH-sorbose reductase

Chain A: 




- Molecule 1: NADPH-sorbose reductase

Chain B: 



- Molecule 1: NADPH-sorbose reductase

Chain H: 



- Molecule 1: NADPH-sorbose reductase

Chain D: 



- Molecule 1: NADPH-sorbose reductase

Chain E: 



- Molecule 1: NADPH-sorbose reductase

Chain C: 



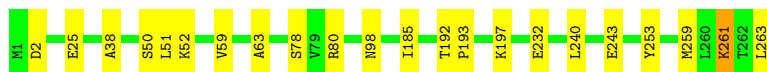
- Molecule 1: NADPH-sorbose reductase

Chain F: 90% 8%



- Molecule 1: NADPH-sorbose reductase

Chain G: 92% 8%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.29Å 60.98Å 124.45Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	19.67 – 1.90 19.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.67-1.90) 99.8 (19.66-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.172 , 0.221 0.173 , 0.221	Depositor DCC
$R_{free}$ test set	7364 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.477 for h,-k,-l 0.000 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17723	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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 71.80 % 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 2.4651e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP

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	0.94	1/2029 (0.0%)	0.83	0/2747
1	B	0.95	0/2029	0.83	1/2747 (0.0%)
1	C	0.91	0/2029	0.78	0/2747
1	D	0.92	1/2029 (0.0%)	0.81	0/2747
1	E	0.92	1/2029 (0.0%)	0.80	1/2747 (0.0%)
1	F	0.90	0/2029	0.82	4/2747 (0.1%)
1	G	0.94	1/2029 (0.0%)	0.81	0/2747
1	H	0.96	1/2029 (0.0%)	0.85	1/2747 (0.0%)
All	All	0.93	5/16232 (0.0%)	0.82	7/21976 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	232	GLU	CB-CG	-5.67	1.41	1.52
1	D	232	GLU	CB-CG	-5.46	1.41	1.52
1	G	232	GLU	CB-CG	-5.28	1.42	1.52
1	A	99	GLU	CB-CG	5.22	1.62	1.52
1	E	162	ALA	CA-CB	5.00	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	132	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	134	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	E	81	SER	CB-CA-C	-5.73	99.22	110.10
1	F	178	ASP	CB-CG-OD1	5.36	123.13	118.30
1	H	244	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	44	LEU	CA-CB-CG	5.03	126.86	115.30
1	F	240	LEU	CB-CG-CD1	-5.02	102.47	111.00

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	1991	0	2000	25	0
1	B	1991	0	2000	21	0
1	C	1991	0	2000	16	0
1	D	1991	0	2000	12	0
1	E	1991	0	2000	14	0
1	F	1991	0	2000	20	0
1	G	1991	0	2000	17	0
1	H	1991	0	2000	25	0
2	A	48	0	26	1	0
2	B	48	0	26	2	0
2	C	48	0	26	2	0
2	D	48	0	26	1	0
2	E	48	0	26	1	0
2	F	48	0	26	2	0
2	G	48	0	26	0	0
2	H	48	0	26	1	0
3	A	183	0	0	4	0
3	B	187	0	0	2	0
3	C	169	0	0	6	0
3	D	179	0	0	1	0
3	E	166	0	0	1	0
3	F	157	0	0	3	0
3	G	169	0	0	5	0
3	H	201	0	0	4	0
All	All	17723	0	16208	141	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 4.

All (141) 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:H:197:LYS:HB3	1:H:197:LYS:NZ	1.30	1.28
1:G:243:GLU:HG3	3:G:4128:HOH:O	1.33	1.20
1:G:261:LYS:HE2	1:G:261:LYS:HA	1.23	1.16
1:G:2:ASP:HB2	3:G:4031:HOH:O	1.46	1.15
1:H:177:LYS:HE3	3:H:290:HOH:O	1.49	1.12
1:H:197:LYS:CB	1:H:197:LYS:HZ2	1.66	1.08
1:H:77:GLU:HG2	3:H:1631:HOH:O	1.66	0.95
1:C:2:ASP:HB3	3:C:275:HOH:O	1.69	0.91
1:G:261:LYS:CA	1:G:261:LYS:HE2	2.09	0.82
1:G:261:LYS:CE	1:G:261:LYS:HA	2.09	0.79
1:H:49:ARG:O	1:H:53:GLU:HG3	1.86	0.76
1:H:2:ASP:HB2	3:H:2249:HOH:O	1.87	0.74
1:H:197:LYS:CB	1:H:197:LYS:NZ	2.19	0.74
1:A:49:ARG:O	1:A:53:GLU:HG3	1.88	0.73
1:D:221:HIS:HD2	3:D:1683:HOH:O	1.72	0.72
1:B:197:LYS:NZ	1:B:197:LYS:HB2	2.04	0.71
1:E:240:LEU:HD11	1:E:253:TYR:CD2	2.26	0.70
1:A:177:LYS:NZ	3:A:2346:HOH:O	2.23	0.70
1:H:194:ASP:O	1:H:198:THR:HG23	1.92	0.69
1:B:25:GLU:HG2	1:B:51:LEU:HD21	1.74	0.68
1:A:43:ARG:HH21	1:A:43:ARG:CB	2.05	0.68
1:D:143:ALA:HB3	1:D:186:ASN:ND2	2.10	0.67
1:F:221:HIS:HD2	3:F:4271:HOH:O	1.79	0.65
1:E:152:TRP:HB3	3:E:708:HOH:O	1.97	0.65
1:E:240:LEU:HD11	1:E:253:TYR:HD2	1.61	0.65
1:G:259:MET:O	1:G:261:LYS:HE3	1.96	0.64
1:E:143:ALA:HB3	1:E:186:ASN:ND2	2.13	0.62
1:B:197:LYS:HZ3	1:B:197:LYS:HB2	1.66	0.60
1:B:206:ASN:HD22	1:B:206:ASN:C	2.04	0.60
1:A:42:ASP:HB3	3:A:580:HOH:O	2.01	0.60
1:A:240:LEU:HD11	1:A:253:TYR:CD2	2.36	0.59
1:F:192:THR:HB	1:F:193:PRO:HD2	1.84	0.59
1:D:240:LEU:HD11	1:D:253:TYR:CD2	2.40	0.57
1:F:253:TYR:HD1	1:G:253:TYR:HD1	1.51	0.57
1:H:197:LYS:HB3	1:H:197:LYS:HZ3	1.55	0.57
1:A:42:ASP:OD1	1:A:43:ARG:N	2.37	0.56
1:B:132:ARG:HE	1:B:178:ASP:CG	2.09	0.56
1:B:49:ARG:NH2	3:B:2227:HOH:O	2.39	0.56
1:F:143:ALA:HB3	1:F:186:ASN:OD1	2.07	0.55
1:B:77:GLU:HG2	3:B:2682:HOH:O	2.05	0.55
1:A:253:TYR:HD1	1:C:253:TYR:HD1	1.55	0.55
1:G:261:LYS:CA	1:G:261:LYS:CE	2.79	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:TYR:HD1	1:D:253:TYR:HD1	1.54	0.54
1:E:197:LYS:HB3	1:E:197:LYS:NZ	2.23	0.54
1:C:143:ALA:HB3	1:C:186:ASN:OD1	2.07	0.53
1:D:15:SER:HB2	1:D:36:LEU:HD22	1.91	0.53
1:H:53:GLU:HB3	3:H:2144:HOH:O	2.09	0.53
1:F:132:ARG:HD3	1:F:178:ASP:CG	2.28	0.53
1:H:42:ASP:O	1:H:46:GLU:HG3	2.09	0.52
1:F:44:LEU:HD13	1:F:61:GLU:HB3	1.89	0.52
1:E:14:GLY:HA2	2:E:270:NDP:H1B	1.91	0.52
1:F:29:LYS:O	1:F:29:LYS:HD2	2.10	0.52
1:C:240:LEU:HD11	1:C:253:TYR:CD2	2.45	0.52
1:D:144:SER:H	1:D:186:ASN:HD22	1.56	0.52
1:F:240:LEU:HD11	1:F:253:TYR:CD2	2.45	0.52
1:H:253:TYR:HD2	1:E:253:TYR:HD1	1.59	0.51
1:H:197:LYS:HB3	1:H:197:LYS:HZ2	0.70	0.51
1:H:206:ASN:C	1:H:206:ASN:HD22	2.14	0.51
1:A:220:GLU:O	1:A:220:GLU:HG2	2.10	0.51
1:C:240:LEU:HD11	1:C:253:TYR:HD2	1.76	0.51
1:F:13:THR:O	1:F:92:ASN:HB3	2.11	0.50
1:C:152:TRP:HB3	3:C:3396:HOH:O	2.11	0.50
1:A:206:ASN:C	1:A:206:ASN:HD22	2.14	0.50
1:A:177:LYS:HE3	3:A:347:HOH:O	2.11	0.50
1:C:231:GLU:HG3	3:C:354:HOH:O	2.11	0.50
1:D:14:GLY:HA2	2:D:270:NDP:H1B	1.92	0.49
1:B:36:LEU:HB3	1:B:44:LEU:HD11	1.95	0.49
1:B:52:LYS:HG3	1:B:59:VAL:HG23	1.95	0.49
1:C:60:LEU:HD21	1:C:78:SER:HB3	1.93	0.49
1:F:43:ARG:HG2	3:F:4375:HOH:O	2.12	0.49
1:C:107:GLU:HG2	3:C:721:HOH:O	2.13	0.49
1:A:132:ARG:NH1	1:A:178:ASP:OD1	2.41	0.48
1:E:197:LYS:HZ3	1:E:197:LYS:HB3	1.76	0.48
1:A:163:ALA:HB2	1:B:163:ALA:HB2	1.95	0.48
1:B:197:LYS:NZ	1:B:197:LYS:CB	2.76	0.48
1:D:143:ALA:HB3	1:D:186:ASN:HD21	1.79	0.48
1:H:185:ILE:HD11	1:H:240:LEU:HD12	1.96	0.48
1:D:201:GLU:O	1:D:204:LYS:HG2	2.13	0.48
1:A:146:CYS:SG	1:A:151:LEU:HD12	2.54	0.48
1:F:76:VAL:HG21	1:F:126:GLY:HA3	1.96	0.47
1:A:177:LYS:CE	3:A:347:HOH:O	2.63	0.47
1:F:263:LEU:HA	1:F:263:LEU:HD23	1.54	0.47
1:G:263:LEU:HA	1:G:263:LEU:HD23	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:MET:O	1:B:261:LYS:HD3	2.15	0.47
1:F:14:GLY:HA2	2:F:270:NDP:H1B	1.96	0.46
1:E:143:ALA:HB3	1:E:186:ASN:HD21	1.77	0.46
1:A:43:ARG:HH21	1:A:43:ARG:HB3	1.79	0.46
1:H:64:VAL:HG11	1:H:74:ALA:HB3	1.97	0.46
2:F:270:NDP:H8A	3:F:6987:HOH:O	2.15	0.46
1:H:262:THR:HG22	1:F:149:GLN:HB2	1.98	0.46
1:C:132:ARG:NH1	3:C:1352:HOH:O	2.49	0.46
1:E:60:LEU:HD21	1:E:78:SER:OG	2.16	0.46
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.58	0.45
1:G:197:LYS:HD2	3:G:5221:HOH:O	2.15	0.45
1:D:263:LEU:HA	1:D:263:LEU:HD23	1.57	0.45
1:G:25:GLU:HG2	1:G:51:LEU:HD21	1.97	0.45
1:B:14:GLY:HA2	2:B:270:NDP:H1B	1.98	0.45
1:H:192:THR:HB	1:H:193:PRO:HD2	1.99	0.45
1:A:253:TYR:HD1	1:C:253:TYR:CD1	2.35	0.45
1:A:14:GLY:HA2	2:A:270:NDP:H1B	1.99	0.45
1:D:128:VAL:N	1:D:129:PRO:CD	2.80	0.45
1:H:263:LEU:HD23	1:H:263:LEU:HA	1.66	0.45
1:H:14:GLY:HA2	2:H:270:NDP:H1B	1.99	0.45
1:G:38:ALA:O	1:G:63:ALA:HA	2.17	0.44
1:H:132:ARG:NH2	1:H:178:ASP:OD1	2.51	0.44
1:G:185:ILE:HD11	1:G:240:LEU:HD12	1.98	0.44
1:A:192:THR:HB	1:A:193:PRO:HD2	2.00	0.44
1:A:42:ASP:O	1:A:46:GLU:HG3	2.17	0.44
1:B:206:ASN:ND2	1:B:206:ASN:C	2.71	0.44
1:E:33:HIS:CE1	1:E:58:ARG:HG3	2.52	0.44
1:A:45:HIS:ND1	1:A:61:GLU:OE2	2.51	0.43
1:H:1:MET:HE2	1:H:1:MET:HB3	1.83	0.43
1:B:192:THR:HB	1:B:193:PRO:HD2	2.00	0.43
1:D:38:ALA:O	1:D:63:ALA:HA	2.18	0.43
1:F:146:CYS:SG	1:F:151:LEU:HD12	2.58	0.43
1:G:261:LYS:HD2	3:G:4042:HOH:O	2.17	0.43
1:C:192:THR:HB	1:C:193:PRO:HD2	1.99	0.43
1:B:38:ALA:O	1:B:63:ALA:HA	2.18	0.43
1:B:66:VAL:HG22	2:B:270:NDP:N1A	2.34	0.42
1:E:144:SER:H	1:E:186:ASN:HD22	1.66	0.42
1:H:253:TYR:HD2	1:E:253:TYR:CD1	2.37	0.42
1:C:66:VAL:HG22	2:C:270:NDP:N1A	2.34	0.42
1:A:114:GLU:HA	1:A:118:MET:HB2	2.01	0.42
1:B:251:SER:HB2	1:B:253:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:GLN:HB2	1:F:262:THR:HG22	2.00	0.42
1:A:220:GLU:OE1	1:A:221:HIS:CD2	2.72	0.42
1:B:185:ILE:HD11	1:B:240:LEU:HD12	2.02	0.42
1:F:15:SER:HB2	1:F:36:LEU:HD22	2.02	0.42
1:H:263:LEU:HD21	1:E:166:MET:HA	2.02	0.42
1:F:240:LEU:HD23	1:F:240:LEU:HA	1.88	0.42
1:G:192:THR:HB	1:G:193:PRO:HD2	2.01	0.42
1:C:14:GLY:HA2	2:C:270:NDP:H1B	2.02	0.41
1:F:192:THR:HB	1:F:193:PRO:CD	2.49	0.41
1:G:52:LYS:HG3	1:G:59:VAL:HG23	2.03	0.41
1:C:122:ARG:NH1	3:C:1671:HOH:O	2.54	0.41
1:F:29:LYS:HA	1:F:29:LYS:HD3	1.80	0.41
1:A:263:LEU:HA	1:A:263:LEU:HD23	1.66	0.41
1:A:43:ARG:HH21	1:A:43:ARG:CG	2.34	0.40
1:A:143:ALA:HB3	1:A:186:ASN:OD1	2.21	0.40
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.64	0.40
1:G:80:ARG:NH2	3:G:4252:HOH:O	2.54	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	261/263 (99%)	256 (98%)	5 (2%)	0	100	100
1	B	261/263 (99%)	253 (97%)	7 (3%)	1 (0%)	38	26
1	C	261/263 (99%)	251 (96%)	9 (3%)	1 (0%)	38	26
1	D	261/263 (99%)	253 (97%)	8 (3%)	0	100	100
1	E	261/263 (99%)	255 (98%)	4 (2%)	2 (1%)	22	11
1	F	261/263 (99%)	249 (95%)	12 (5%)	0	100	100
1	G	261/263 (99%)	255 (98%)	5 (2%)	1 (0%)	38	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	261/263 (99%)	256 (98%)	5 (2%)	0	100	100
All	All	2088/2104 (99%)	2028 (97%)	55 (3%)	5 (0%)	51	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	98	ASN
1	E	144	SER
1	C	98	ASN
1	G	98	ASN
1	B	98	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	206/206 (100%)	202 (98%)	4 (2%)	62	57
1	B	206/206 (100%)	201 (98%)	5 (2%)	54	47
1	C	206/206 (100%)	202 (98%)	4 (2%)	62	57
1	D	206/206 (100%)	201 (98%)	5 (2%)	54	47
1	E	206/206 (100%)	204 (99%)	2 (1%)	80	80
1	F	206/206 (100%)	202 (98%)	4 (2%)	62	57
1	G	206/206 (100%)	203 (98%)	3 (2%)	70	67
1	H	206/206 (100%)	201 (98%)	5 (2%)	54	47
All	All	1648/1648 (100%)	1616 (98%)	32 (2%)	62	57

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	142	ASN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	236	PHE
1	B	40	GLN
1	B	50	SER
1	B	204	LYS
1	B	206	ASN
1	B	261	LYS
1	H	49	ARG
1	H	50	SER
1	H	197	LYS
1	H	198	THR
1	H	206	ASN
1	D	50	SER
1	D	51	LEU
1	D	54	LYS
1	D	193	PRO
1	D	197	LYS
1	E	46	GLU
1	E	50	SER
1	C	5	ILE
1	C	41	VAL
1	C	193	PRO
1	C	197	LYS
1	F	44	LEU
1	F	193	PRO
1	F	197	LYS
1	F	216	SER
1	G	50	SER
1	G	78	SER
1	G	261	LYS

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	142	ASN
1	A	206	ASN
1	B	206	ASN
1	H	45	HIS
1	H	206	ASN
1	D	186	ASN
1	D	221	HIS
1	E	186	ASN

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Mol	Chain	Res	Type
1	F	141	HIS
1	F	221	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NDP	A	270	-	43,52,52	1.69	5 (11%)	49,80,80	2.09	5 (10%)
2	NDP	B	270	-	43,52,52	1.68	5 (11%)	49,80,80	1.72	4 (8%)
2	NDP	C	270	-	43,52,52	1.59	6 (13%)	49,80,80	2.05	7 (14%)
2	NDP	D	270	-	43,52,52	1.61	5 (11%)	49,80,80	2.07	4 (8%)
2	NDP	E	270	-	43,52,52	1.56	5 (11%)	49,80,80	1.84	5 (10%)
2	NDP	F	270	-	43,52,52	1.59	5 (11%)	49,80,80	2.00	5 (10%)
2	NDP	G	270	-	43,52,52	1.69	5 (11%)	49,80,80	1.71	4 (8%)
2	NDP	H	270	-	43,52,52	1.65	5 (11%)	49,80,80	2.19	5 (10%)

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	NDP	A	270	-	-	0/30/77/77	0/5/5/5
2	NDP	B	270	-	-	0/30/77/77	0/5/5/5
2	NDP	C	270	-	-	0/30/77/77	0/5/5/5
2	NDP	D	270	-	-	0/30/77/77	0/5/5/5
2	NDP	E	270	-	-	0/30/77/77	0/5/5/5
2	NDP	F	270	-	-	0/30/77/77	0/5/5/5
2	NDP	G	270	-	-	0/30/77/77	0/5/5/5
2	NDP	H	270	-	-	0/30/77/77	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	270	NDP	C4N-C5N	-3.89	1.40	1.49
2	E	270	NDP	C4N-C5N	-3.88	1.40	1.49
2	C	270	NDP	C4N-C5N	-3.85	1.40	1.49
2	H	270	NDP	C4N-C5N	-3.77	1.40	1.49
2	F	270	NDP	C4N-C5N	-3.50	1.41	1.49
2	A	270	NDP	C4N-C5N	-3.36	1.41	1.49
2	G	270	NDP	C4N-C5N	-3.33	1.41	1.49
2	D	270	NDP	C4N-C5N	-3.08	1.42	1.49
2	H	270	NDP	C2A-N1A	2.11	1.37	1.33
2	F	270	NDP	C2A-N1A	2.17	1.38	1.33
2	B	270	NDP	C2A-N1A	2.23	1.38	1.33
2	D	270	NDP	P2B-O2B	2.32	1.63	1.59
2	C	270	NDP	C2A-N1A	2.37	1.38	1.33
2	C	270	NDP	P2B-O2B	2.39	1.63	1.59
2	A	270	NDP	C2A-N1A	2.49	1.38	1.33
2	E	270	NDP	C2A-N1A	2.55	1.38	1.33
2	G	270	NDP	C2A-N1A	3.12	1.39	1.33
2	F	270	NDP	C6N-C5N	3.47	1.39	1.33
2	G	270	NDP	C6N-C5N	3.61	1.40	1.33
2	E	270	NDP	C2A-N3A	3.62	1.38	1.32
2	C	270	NDP	C2A-N3A	3.88	1.38	1.32
2	D	270	NDP	C6N-C5N	3.98	1.40	1.33
2	D	270	NDP	C2A-N3A	4.16	1.39	1.32
2	F	270	NDP	C2A-N3A	4.18	1.39	1.32
2	C	270	NDP	C6N-C5N	4.25	1.41	1.33
2	B	270	NDP	C6N-C5N	4.26	1.41	1.33
2	H	270	NDP	C2A-N3A	4.31	1.39	1.32
2	E	270	NDP	C6N-C5N	4.36	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	270	NDP	C6N-C5N	4.53	1.41	1.33
2	G	270	NDP	C2A-N3A	4.55	1.39	1.32
2	A	270	NDP	C2A-N3A	4.62	1.39	1.32
2	B	270	NDP	C2A-N3A	4.68	1.40	1.32
2	H	270	NDP	C6N-C5N	4.90	1.42	1.33
2	C	270	NDP	O7N-C7N	5.26	1.37	1.24
2	E	270	NDP	O7N-C7N	5.44	1.38	1.24
2	H	270	NDP	O7N-C7N	5.82	1.39	1.24
2	B	270	NDP	O7N-C7N	6.01	1.39	1.24
2	D	270	NDP	O7N-C7N	6.10	1.39	1.24
2	A	270	NDP	O7N-C7N	6.18	1.39	1.24
2	G	270	NDP	O7N-C7N	6.26	1.40	1.24
2	F	270	NDP	O7N-C7N	6.46	1.40	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	270	NDP	N3A-C2A-N1A	-12.87	117.65	128.86
2	A	270	NDP	N3A-C2A-N1A	-12.10	118.32	128.86
2	D	270	NDP	N3A-C2A-N1A	-11.95	118.45	128.86
2	F	270	NDP	N3A-C2A-N1A	-11.82	118.56	128.86
2	C	270	NDP	N3A-C2A-N1A	-10.61	119.62	128.86
2	E	270	NDP	N3A-C2A-N1A	-9.83	120.30	128.86
2	B	270	NDP	N3A-C2A-N1A	-9.54	120.55	128.86
2	G	270	NDP	N3A-C2A-N1A	-9.00	121.02	128.86
2	C	270	NDP	C1B-N9A-C4A	-3.98	119.76	126.64
2	G	270	NDP	C3N-C2N-N1N	-3.57	117.90	123.08
2	H	270	NDP	C1B-N9A-C4A	-3.53	120.54	126.64
2	B	270	NDP	C3N-C2N-N1N	-3.44	118.08	123.08
2	A	270	NDP	C1B-N9A-C4A	-3.42	120.73	126.64
2	C	270	NDP	C3N-C2N-N1N	-3.23	118.40	123.08
2	G	270	NDP	C1B-N9A-C4A	-3.17	121.16	126.64
2	C	270	NDP	C4B-O4B-C1B	-2.77	106.82	109.77
2	E	270	NDP	C3N-C2N-N1N	-2.77	119.07	123.08
2	E	270	NDP	C1B-N9A-C4A	-2.72	121.94	126.64
2	F	270	NDP	C1B-N9A-C4A	-2.62	122.11	126.64
2	F	270	NDP	C3N-C2N-N1N	-2.59	119.32	123.08
2	A	270	NDP	C3N-C2N-N1N	-2.34	119.68	123.08
2	D	270	NDP	C3N-C2N-N1N	-2.30	119.73	123.08
2	E	270	NDP	O2B-P2B-O1X	-2.22	100.58	109.26
2	D	270	NDP	O2B-P2B-O1X	-2.19	100.67	109.26
2	E	270	NDP	C1D-N1N-C2N	-2.12	117.48	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	270	NDP	O2B-P2B-O1X	-2.11	101.01	109.26
2	A	270	NDP	O2X-P2B-O1X	-2.07	102.40	110.50
2	F	270	NDP	C2A-N1A-C6A	2.04	122.33	118.77
2	C	270	NDP	O4B-C4B-C3B	2.07	109.28	105.17
2	H	270	NDP	O2D-C2D-C1D	2.11	117.07	109.96
2	B	270	NDP	O2D-C2D-C1D	2.18	117.32	109.96
2	G	270	NDP	O2N-PN-O1N	2.19	123.64	112.28
2	B	270	NDP	O2N-PN-O1N	2.29	124.16	112.28
2	A	270	NDP	O2N-PN-O1N	2.39	124.66	112.28
2	H	270	NDP	C2A-N1A-C6A	2.43	123.02	118.77
2	D	270	NDP	O3X-P2B-O1X	2.55	120.46	110.50
2	H	270	NDP	O2N-PN-O1N	2.61	125.78	112.28
2	C	270	NDP	O2B-C2B-C1B	2.61	119.81	110.06
2	F	270	NDP	O3X-P2B-O2X	3.12	120.22	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	270	NDP	1	0
2	B	270	NDP	2	0
2	C	270	NDP	2	0
2	D	270	NDP	1	0
2	E	270	NDP	1	0
2	F	270	NDP	2	0
2	H	270	NDP	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	263/263 (100%)	-0.51	1 (0%) 92 93	9, 16, 28, 41	0
1	B	263/263 (100%)	-0.46	0 100 100	9, 16, 31, 44	0
1	C	263/263 (100%)	-0.47	0 100 100	10, 17, 32, 39	0
1	D	263/263 (100%)	-0.49	0 100 100	10, 17, 32, 37	0
1	E	263/263 (100%)	-0.47	0 100 100	10, 17, 33, 37	0
1	F	263/263 (100%)	-0.48	1 (0%) 92 93	10, 17, 33, 38	0
1	G	263/263 (100%)	-0.48	0 100 100	9, 17, 30, 43	0
1	H	263/263 (100%)	-0.51	1 (0%) 92 93	9, 16, 28, 39	0
All	All	2104/2104 (100%)	-0.48	3 (0%) 95 95	9, 17, 32, 44	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	45	HIS	2.4
1	A	45	HIS	2.3
1	F	194	ASP	2.1

### 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

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NDP	E	270	48/48	0.94	0.12	0.88	14,21,25,27	0
2	NDP	D	270	48/48	0.96	0.10	0.51	16,22,25,26	0
2	NDP	C	270	48/48	0.96	0.09	0.02	15,21,25,27	0
2	NDP	B	270	48/48	0.97	0.08	-0.03	12,19,23,25	0
2	NDP	F	270	48/48	0.96	0.08	-0.06	17,22,26,29	0
2	NDP	G	270	48/48	0.97	0.08	-0.14	13,19,23,25	0
2	NDP	A	270	48/48	0.96	0.09	-0.14	13,20,27,27	0
2	NDP	H	270	48/48	0.97	0.08	-0.27	13,21,24,27	0

## 6.5 Other polymers

There are no such residues in this entry.