



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:54 PM GMT

PDB ID : 2GCG  
Title : Ternary Crystal Structure of Human Glyoxylate Reductase/Hydroxypyruvate Reductase  
Authors : Booth, M.P.S.; Connors, R.; Rumsby, G.; Brady, R.L.  
Deposited on : 2006-03-14  
Resolution : 2.20 Å(reported)

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

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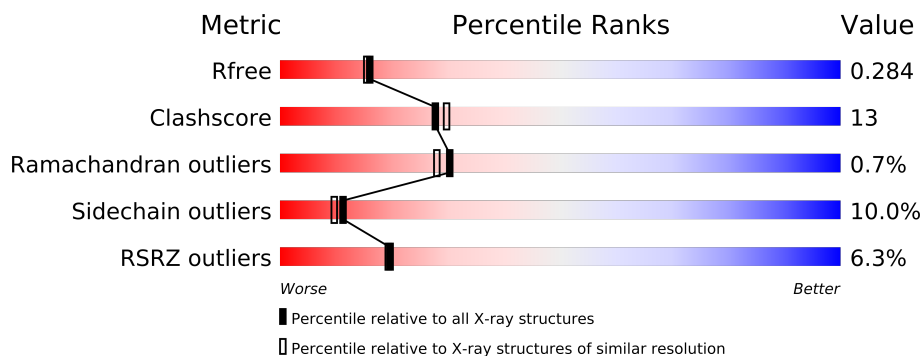
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	330	
1	B	330	
1	C	330	
1	D	330	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	C	1001	-	X
2	SO4	D	1002	-	X
2	SO4	D	1003	-	X
3	NDP	B	2002	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	NDP	D	2004	-	X
4	DGY	C	3002	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10701 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 Glyoxylate reductase/hydroxypyruvatereductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2471	1560	438	461	12			
1	B	323	Total	C	N	O	S	0	0	0
			2459	1554	434	459	12			
1	C	324	Total	C	N	O	S	0	0	0
			2470	1560	438	460	12			
1	D	323	Total	C	N	O	S	0	0	0
			2459	1554	434	459	12			

There are 8 discrepancies between the modelled and reference sequences:

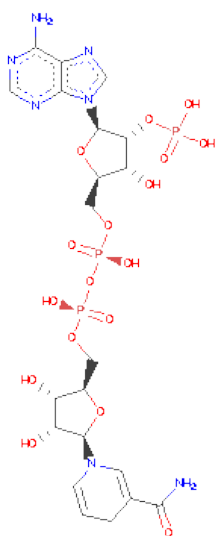
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	CLONING ARTIFACT	UNP Q9UBQ7
A	0	SER	-	CLONING ARTIFACT	UNP Q9UBQ7
B	-1	ALA	-	CLONING ARTIFACT	UNP Q9UBQ7
B	0	SER	-	CLONING ARTIFACT	UNP Q9UBQ7
C	-1	ALA	-	CLONING ARTIFACT	UNP Q9UBQ7
C	0	SER	-	CLONING ARTIFACT	UNP Q9UBQ7
D	-1	ALA	-	CLONING ARTIFACT	UNP Q9UBQ7
D	0	SER	-	CLONING ARTIFACT	UNP Q9UBQ7

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



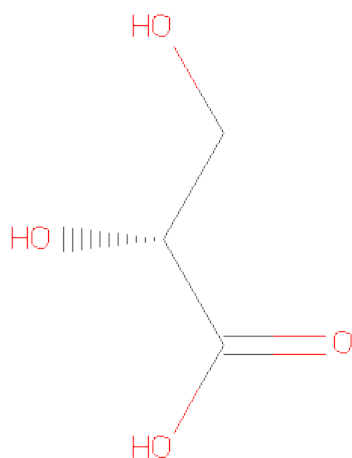
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (2R)-2,3-DIHYDROXYPROPANOICACID (three-letter code: DGY) (formula:  $C_3H_6O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is water.

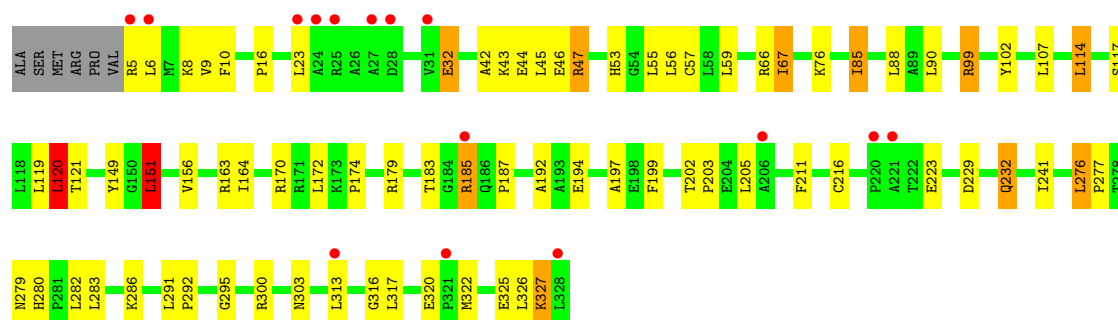
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		
5	B	182	Total	O	0	0
			182	182		
5	C	132	Total	O	0	0
			132	132		
5	D	129	Total	O	0	0
			129	129		

### 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.

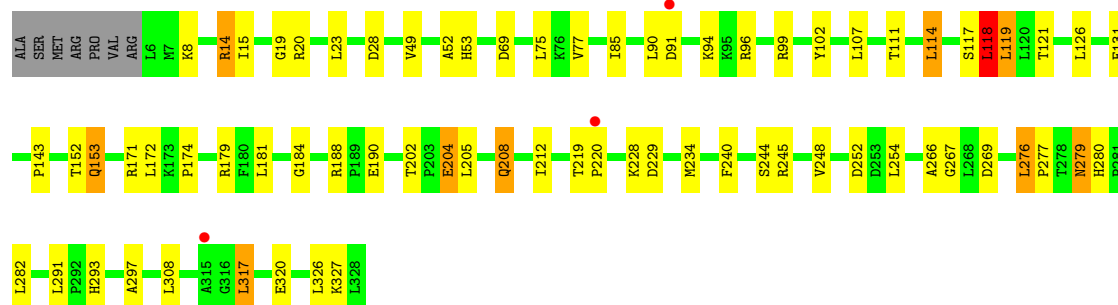
- Molecule 1: Glyoxylate reductase/hydroxypyruvatereductase

Chain A: 



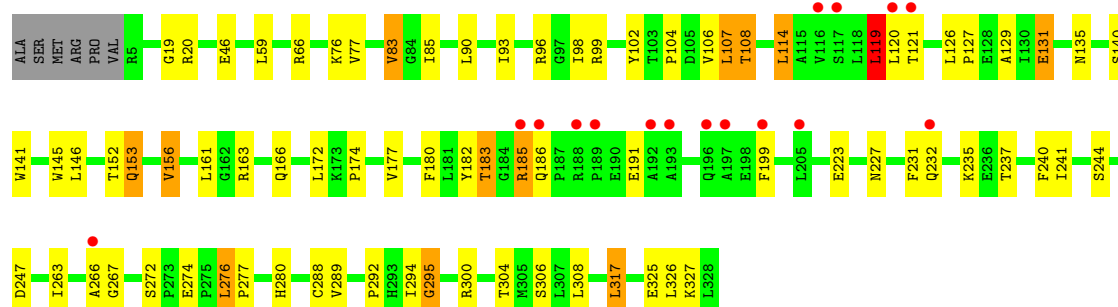
- Molecule 1: Glyoxylate reductase/hydroxypyruvatereductase

Chain B: 



- Molecule 1: Glyoxylate reductase/hydroxypyruvatereductase

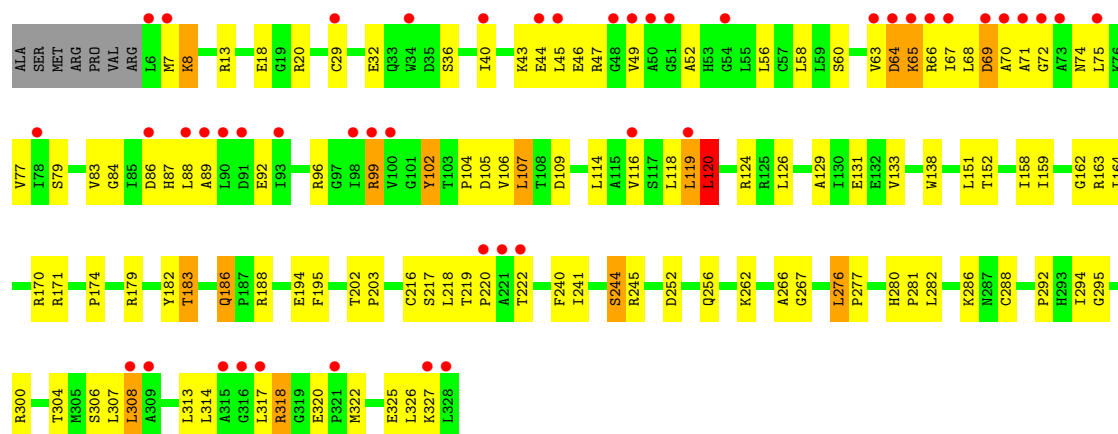
Chain C: 





● Molecule 1: Glyoxylate reductase/hydroxypyruvatereductase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.57Å 66.88Å 149.78Å 90.00° 98.22° 90.00°	Depositor
Resolution (Å)	46.20 – 2.20 46.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.0 (46.20-2.20) 90.0 (46.19-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.201 , 0.282 0.205 , 0.284	Depositor DCC
$R_{free}$ test set	3459 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 69056 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, DGY, 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	0.77	0/2515	0.88	9/3414 (0.3%)
1	B	0.83	0/2503	0.89	7/3400 (0.2%)
1	C	0.74	0/2514	0.84	2/3414 (0.1%)
1	D	0.80	4/2503 (0.2%)	0.88	7/3400 (0.2%)
All	All	0.78	4/10035 (0.0%)	0.87	25/13628 (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	B	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	ASP	CG-OD1	8.31	1.44	1.25
1	D	8	LYS	CE-NZ	8.12	1.69	1.49
1	D	69	ASP	CG-OD2	6.96	1.41	1.25
1	D	318	ARG	CZ-NH2	5.49	1.40	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	LEU	CA-CB-CG	8.61	135.10	115.30
1	A	276	LEU	CA-CB-CG	7.74	133.11	115.30
1	C	119	LEU	CA-CB-CG	7.41	132.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	LEU	CA-CB-CG	-6.69	99.91	115.30
1	B	119	LEU	CA-CB-CG	6.33	129.85	115.30
1	A	120	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	205	LEU	CA-CB-CG	6.17	129.48	115.30
1	B	171	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	114	LEU	CA-CB-CG	-5.94	101.63	115.30
1	B	14	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	114	LEU	CA-CB-CG	-5.84	101.87	115.30
1	A	151	LEU	CA-CB-CG	5.83	128.71	115.30
1	D	318	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	69	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	276	LEU	CB-CG-CD2	5.48	120.31	111.00
1	B	119	LEU	CB-CG-CD1	5.33	120.06	111.00
1	A	99	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	124	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	D	120	LEU	CB-CG-CD1	5.19	119.82	111.00
1	B	118	LEU	CB-CG-CD2	5.15	119.75	111.00
1	A	114	LEU	CB-CG-CD2	5.12	119.71	111.00
1	D	126	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	120	LEU	CB-CG-CD1	5.08	119.64	111.00
1	D	120	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	114	LEU	CB-CG-CD2	5.04	119.56	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	ALA	Peptide
1	D	64	ASP	Peptide

## 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	2471	0	2528	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2459	0	2515	41	1
1	C	2470	0	2528	63	1
1	D	2459	0	2515	101	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	15	0	0	0	0
3	A	48	0	26	10	0
3	B	48	0	26	2	0
3	C	48	0	26	4	0
3	D	48	0	26	10	0
4	A	7	0	5	7	0
4	C	7	0	5	4	0
5	A	168	0	0	7	0
5	B	182	0	0	2	0
5	C	132	0	0	5	0
5	D	129	0	0	2	0
All	All	10701	0	10200	260	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (260) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:8:LYS:CE	1:D:8:LYS:NZ	1.69	1.56
1:D:63:VAL:HG21	1:D:88:LEU:CD2	1.47	1.42
1:D:64:ASP:CB	1:D:65:LYS:HB2	1.49	1.41
1:D:64:ASP:HB2	1:D:65:LYS:CB	1.55	1.36
1:D:63:VAL:CG2	1:D:88:LEU:CD2	2.03	1.35
1:D:63:VAL:CG2	1:D:88:LEU:HD23	1.64	1.20
1:D:63:VAL:CB	1:D:88:LEU:HD23	1.76	1.14
1:D:114:LEU:HD11	1:D:294:ILE:HG13	1.31	1.08
1:D:63:VAL:HB	1:D:88:LEU:HD23	1.35	1.07
3:C:2003:NDP:H42N	4:C:3002:DGY:H2	1.37	1.05
1:D:63:VAL:CB	1:D:88:LEU:CD2	2.35	1.01
1:A:149:TYR:HD1	5:A:3166:HOH:O	1.43	1.00
1:D:8:LYS:HE3	1:D:32:GLU:OE1	1.62	0.98
1:A:163:ARG:HG2	5:A:3010:HOH:O	1.62	0.98
3:A:2001:NDP:C4N	4:A:3001:DGY:H2	1.93	0.97
1:D:64:ASP:OD2	1:D:66:ARG:HG2	1.65	0.96
1:D:63:VAL:CG2	1:D:88:LEU:HD21	1.79	0.93
3:C:2003:NDP:C4N	4:C:3002:DGY:H2	1.99	0.93
3:A:2001:NDP:H42N	4:A:3001:DGY:H2	1.49	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:ARG:NH1	1:B:153:GLN:HG2	1.84	0.92
1:A:47:ARG:HG3	1:A:47:ARG:HH11	1.32	0.91
1:D:63:VAL:HG21	1:D:88:LEU:HD21	0.91	0.90
1:D:63:VAL:HB	1:D:88:LEU:CD2	2.00	0.88
1:C:85:ILE:HD13	1:C:90:LEU:HD11	1.56	0.87
1:C:183:THR:HG22	3:C:2003:NDP:H2A	1.58	0.85
1:D:64:ASP:CA	1:D:65:LYS:HB2	2.06	0.85
1:D:8:LYS:CE	1:D:32:GLU:OE1	2.24	0.85
1:D:77:VAL:HG21	1:D:322:MET:CE	2.10	0.81
1:D:106:VAL:CG2	1:D:304:THR:HG22	2.11	0.80
1:D:164:ILE:HD12	3:D:2004:NDP:H51N	1.63	0.78
1:C:153:GLN:HE21	1:C:153:GLN:HA	1.48	0.78
3:A:2001:NDP:O1A	5:A:3021:HOH:O	2.01	0.77
1:D:106:VAL:HG21	1:D:304:THR:HG22	1.67	0.77
1:A:174:PRO:HG3	1:B:174:PRO:HG3	1.65	0.76
1:D:13:ARG:HG2	1:D:36:SER:O	1.86	0.75
1:D:63:VAL:HG23	1:D:88:LEU:HD23	1.65	0.74
1:B:69:ASP:OD2	1:B:96:ARG:NH2	2.21	0.74
1:D:314:LEU:O	1:D:318:ARG:HD2	1.88	0.73
1:D:114:LEU:HD13	1:D:295:GLY:HA2	1.69	0.73
1:D:280:HIS:HD2	1:D:282:LEU:H	1.37	0.72
1:D:77:VAL:HG21	1:D:322:MET:HE1	1.71	0.72
1:D:202:THR:OG1	1:D:203:PRO:HD3	1.89	0.71
1:D:114:LEU:CD1	1:D:294:ILE:HG13	2.17	0.70
1:C:108:THR:HG21	5:C:3006:HOH:O	1.90	0.70
3:D:2004:NDP:O1X	5:D:2107:HOH:O	2.10	0.69
1:A:47:ARG:CG	1:A:47:ARG:HH11	2.04	0.69
1:A:164:ILE:HD12	3:A:2001:NDP:H51N	1.73	0.69
1:C:241:ILE:HD13	1:C:267:GLY:HA2	1.76	0.68
1:C:276:LEU:HD22	1:C:277:PRO:HD2	1.75	0.68
1:C:174:PRO:HG3	1:D:174:PRO:HG3	1.76	0.68
1:D:45:LEU:O	1:D:49:VAL:HG22	1.93	0.68
1:D:106:VAL:HG23	1:D:304:THR:CG2	2.23	0.68
1:C:266:ALA:O	1:C:288:CYS:HA	1.94	0.67
1:C:106:VAL:HG11	1:C:304:THR:HG22	1.76	0.67
1:B:152:THR:OG1	5:B:2038:HOH:O	2.13	0.67
1:C:83:VAL:HG22	1:C:107:LEU:HD21	1.77	0.67
1:D:241:ILE:HD13	1:D:267:GLY:HA2	1.75	0.66
1:D:106:VAL:CG2	1:D:304:THR:CG2	2.73	0.66
1:A:59:LEU:CD2	4:A:3001:DGy:H3C2	2.26	0.66
1:B:8:LYS:H	1:B:53:HIS:HD2	1.43	0.65
1:B:212:ILE:HD12	1:B:234:MET:CE	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:HIS:HE1	5:A:3103:HOH:O	1.79	0.65
1:C:235:LYS:HB3	1:C:237:THR:HG22	1.78	0.65
1:A:10:PHE:HD2	1:A:32:GLU:HG2	1.62	0.64
1:D:64:ASP:HB2	1:D:65:LYS:HB2	0.73	0.64
1:D:280:HIS:CD2	1:D:282:LEU:H	2.15	0.64
1:B:280:HIS:HD2	1:B:282:LEU:H	1.46	0.64
1:D:69:ASP:OD1	1:D:96:ARG:NH2	2.31	0.64
1:D:188:ARG:NH2	3:D:2004:NDP:O3B	2.31	0.64
1:A:76:LYS:NZ	1:A:316:GLY:O	2.31	0.64
1:D:64:ASP:OD2	1:D:66:ARG:CG	2.45	0.62
1:D:162:GLY:HA3	3:D:2004:NDP:O1A	1.99	0.62
1:D:114:LEU:CD1	1:D:294:ILE:O	2.47	0.62
1:A:170:ARG:HD3	1:A:194:GLU:OE2	1.99	0.62
3:A:2001:NDP:C5N	4:A:3001:DGY:H2	2.29	0.61
1:A:300:ARG:HH12	1:B:153:GLN:HG2	1.62	0.61
1:A:99:ARG:HD2	1:A:325:GLU:OE1	2.00	0.61
1:B:8:LYS:H	1:B:53:HIS:CD2	2.18	0.61
1:A:121:THR:HG21	1:B:126:LEU:HD22	1.82	0.61
1:C:276:LEU:CD2	1:C:277:PRO:HD2	2.31	0.61
1:C:83:VAL:HG13	1:C:104:PRO:HA	1.80	0.61
3:A:2001:NDP:C3N	4:A:3001:DGY:H2	2.29	0.61
1:D:114:LEU:HD13	1:D:295:GLY:CA	2.31	0.60
1:A:185:ARG:HD3	3:A:2001:NDP:O3X	2.01	0.60
1:D:77:VAL:CG2	1:D:322:MET:HE1	2.30	0.60
1:D:83:VAL:HG11	3:D:2004:NDP:H6N	1.83	0.60
1:D:29:CYS:SG	1:D:317:LEU:CD2	2.90	0.60
1:C:140:SER:OG	1:C:141:TRP:N	2.35	0.60
1:D:63:VAL:CB	1:D:88:LEU:HD22	2.31	0.59
3:C:2003:NDP:C3N	4:C:3002:DGY:H2	2.32	0.59
1:C:83:VAL:HG22	1:C:107:LEU:HD11	1.84	0.59
1:D:216:CYS:O	1:D:244:SER:HB2	2.02	0.59
1:B:279:ASN:HD22	1:B:279:ASN:H	1.51	0.59
1:A:119:LEU:HD13	1:A:241:ILE:HG13	1.84	0.59
1:A:85:ILE:HG12	1:A:326:LEU:HD22	1.85	0.59
1:D:116:VAL:HG12	1:D:120:LEU:HD22	1.85	0.58
1:B:114:LEU:O	1:B:114:LEU:HG	2.03	0.58
1:B:280:HIS:CD2	1:B:282:LEU:H	2.22	0.58
1:D:106:VAL:HG23	1:D:304:THR:HG21	1.86	0.57
1:C:99:ARG:HD2	1:C:325:GLU:OE1	2.04	0.57
1:A:286:LYS:HG2	5:A:3002:HOH:O	2.03	0.57
1:C:300:ARG:NH2	1:D:152:THR:HG23	2.20	0.57
1:A:119:LEU:HD11	1:A:211:PHE:CD1	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:153:GLN:NE2	1:C:153:GLN:HA	2.19	0.56
1:D:106:VAL:HG23	1:D:304:THR:HG22	1.85	0.56
1:A:119:LEU:HD11	1:A:211:PHE:HD1	1.70	0.55
3:D:2004:NDP:H6N	3:D:2004:NDP:H3D	1.88	0.55
1:C:300:ARG:HH21	1:D:152:THR:HG23	1.71	0.55
1:C:108:THR:HG22	5:C:3008:HOH:O	2.05	0.55
1:D:43:LYS:O	1:D:46:GLU:HB3	2.06	0.55
1:C:83:VAL:CG2	1:C:107:LEU:HD11	2.37	0.55
1:C:114:LEU:HD22	1:C:295:GLY:HA2	1.88	0.55
1:B:179:ARG:NE	1:B:181:LEU:HD21	2.21	0.54
1:D:99:ARG:NH2	1:D:320:GLU:O	2.36	0.54
1:C:161:LEU:HG	1:C:166:GLN:HG3	1.90	0.54
1:A:9:VAL:CG1	1:A:313:LEU:HD21	2.37	0.54
1:D:159:ILE:HA	1:D:183:THR:HG22	1.90	0.54
1:C:129:ALA:HB1	1:D:292:PRO:HD2	1.90	0.54
1:C:114:LEU:CD2	1:C:295:GLY:HA2	2.37	0.53
1:D:70:ALA:HA	1:D:71:ALA:C	2.29	0.53
1:B:204:GLU:O	1:B:208:GLN:HG2	2.07	0.53
1:D:8:LYS:CD	1:D:8:LYS:NZ	2.67	0.53
1:B:49:VAL:HG22	1:B:49:VAL:O	2.08	0.53
1:C:266:ALA:O	1:C:289:VAL:N	2.41	0.52
1:D:170:ARG:HD3	1:D:194:GLU:OE2	2.09	0.52
1:A:185:ARG:NH1	3:A:2001:NDP:O2X	2.41	0.52
1:B:118:LEU:HG	1:B:291:LEU:CD1	2.40	0.52
1:C:77:VAL:CG1	1:C:317:LEU:HD13	2.40	0.52
1:D:8:LYS:HE2	1:D:32:GLU:OE1	2.08	0.52
3:D:2004:NDP:O1A	3:D:2004:NDP:O1N	2.27	0.52
1:B:245:ARG:O	1:B:248:VAL:HG22	2.10	0.52
1:A:9:VAL:HG13	1:A:313:LEU:HD21	1.91	0.52
1:A:117:SER:O	1:A:121:THR:HG23	2.10	0.51
1:A:151:LEU:HD13	1:A:211:PHE:CE2	2.45	0.51
1:C:185:ARG:HD2	1:C:186:GLN:HB3	1.92	0.51
1:A:291:LEU:HB3	1:A:292:PRO:HD2	1.92	0.51
1:D:44:GLU:OE1	1:D:47:ARG:NH2	2.43	0.51
1:C:274:GLU:HG2	1:D:138:TRP:CZ2	2.45	0.51
1:C:114:LEU:HD22	1:C:295:GLY:N	2.26	0.51
1:D:102:TYR:CZ	1:D:104:PRO:HG3	2.45	0.51
1:D:322:MET:SD	1:D:325:GLU:HB3	2.51	0.51
1:D:276:LEU:HD22	1:D:277:PRO:HD2	1.93	0.50
1:B:99:ARG:NH2	1:B:320:GLU:O	2.32	0.50
1:D:114:LEU:HD13	1:D:294:ILE:O	2.11	0.50
1:D:266:ALA:O	1:D:288:CYS:HA	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:GLU:OE2	1:A:47:ARG:NH2	2.46	0.49
1:C:119:LEU:HB2	1:C:241:ILE:HG13	1.93	0.49
1:D:83:VAL:HB	1:D:107:LEU:HD11	1.94	0.49
1:D:68:LEU:O	1:D:72:GLY:HA2	2.13	0.49
1:A:119:LEU:HD13	1:A:241:ILE:CG1	2.42	0.49
1:D:295:GLY:HA3	3:D:2004:NDP:O7N	2.13	0.49
1:B:276:LEU:HD22	1:B:277:PRO:HD2	1.94	0.48
1:C:46:GLU:CD	1:C:66:ARG:HD3	2.33	0.48
1:A:8:LYS:H	1:A:53:HIS:HD2	1.62	0.48
1:D:64:ASP:HB2	1:D:65:LYS:HB3	1.78	0.48
1:A:121:THR:HG21	1:B:126:LEU:CD2	2.42	0.48
1:C:114:LEU:HD22	1:C:295:GLY:CA	2.43	0.48
1:B:184:GLY:HA2	3:B:2002:NDP:C2A	2.43	0.48
1:A:114:LEU:HG	1:A:114:LEU:O	2.09	0.48
1:B:219:THR:HB	1:B:220:PRO:HD2	1.95	0.48
1:C:156:VAL:HG13	1:C:177:VAL:HG13	1.94	0.48
1:C:235:LYS:C	1:C:237:THR:H	2.16	0.48
1:D:240:PHE:O	1:D:267:GLY:HA3	2.14	0.48
1:B:8:LYS:HG3	1:B:52:ALA:HA	1.96	0.48
1:D:83:VAL:CG1	3:D:2004:NDP:H6N	2.44	0.47
1:A:156:VAL:HG22	1:A:211:PHE:HB2	1.95	0.47
1:A:322:MET:HB2	1:A:325:GLU:HB2	1.96	0.47
1:D:114:LEU:HD13	1:D:294:ILE:C	2.35	0.47
1:D:276:LEU:HD22	1:D:277:PRO:CD	2.44	0.47
1:C:59:LEU:CD2	4:C:3002:DGy:H3C2	2.45	0.46
1:A:280:HIS:HD2	1:A:282:LEU:HB2	1.81	0.46
1:D:159:ILE:HG23	1:D:183:THR:CG2	2.45	0.46
1:C:156:VAL:HG22	1:C:180:PHE:CD2	2.50	0.46
1:D:56:LEU:HA	1:D:79:SER:O	2.15	0.46
1:C:280:HIS:HE1	5:C:3041:HOH:O	1.98	0.46
1:A:202:THR:HB	1:A:203:PRO:HD3	1.97	0.46
1:B:85:ILE:HD13	1:B:90:LEU:HD11	1.96	0.46
1:B:188:ARG:NH2	5:B:2045:HOH:O	2.48	0.46
1:D:114:LEU:C	1:D:114:LEU:HD23	2.36	0.46
1:D:218:LEU:HA	1:D:222:THR:OG1	2.16	0.46
1:C:163:ARG:HD3	5:C:3006:HOH:O	2.15	0.46
1:C:294:ILE:O	1:C:295:GLY:C	2.54	0.46
1:B:118:LEU:HG	1:B:291:LEU:HD11	1.99	0.45
1:D:186:GLN:HE21	1:D:186:GLN:HB3	1.56	0.45
1:A:327:LYS:HB3	1:A:327:LYS:NZ	2.30	0.45
1:D:63:VAL:HG11	1:D:88:LEU:HD22	1.97	0.45
3:D:2004:NDP:C3D	3:D:2004:NDP:H6N	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:29:CYS:SG	1:D:317:LEU:HD22	2.57	0.45
1:B:15:ILE:O	1:B:20:ARG:HD3	2.16	0.45
1:A:47:ARG:HG3	1:A:47:ARG:NH1	2.14	0.45
1:D:83:VAL:HG13	1:D:84:GLY:N	2.31	0.45
1:C:223:GLU:HG3	1:C:247:ASP:HB3	1.99	0.45
1:D:64:ASP:CB	1:D:65:LYS:CB	2.44	0.44
1:A:187:PRO:HG3	1:A:199:PHE:CD1	2.53	0.44
1:A:99:ARG:NH2	1:A:320:GLU:O	2.41	0.44
1:C:153:GLN:HB2	1:D:300:ARG:HH22	1.82	0.44
1:B:77:VAL:HG12	1:B:317:LEU:HD13	2.00	0.44
1:A:42:ALA:O	1:A:46:GLU:HG3	2.18	0.44
1:D:18:GLU:OE2	1:D:307:LEU:HD22	2.18	0.44
1:A:47:ARG:CG	1:A:47:ARG:NH1	2.72	0.43
1:D:218:LEU:HB2	1:D:245:ARG:HB2	2.00	0.43
3:A:2001:NDP:H42N	4:A:3001:DGY:C2	2.34	0.43
1:C:266:ALA:HB1	1:C:267:GLY:HA3	1.99	0.43
1:C:106:VAL:CG1	1:C:304:THR:HG22	2.47	0.43
1:B:28:ASP:OD1	1:B:28:ASP:N	2.51	0.43
1:D:83:VAL:CG1	1:D:84:GLY:N	2.81	0.43
1:D:314:LEU:HB3	1:D:318:ARG:NH1	2.32	0.43
1:C:129:ALA:HA	1:C:146:LEU:CD1	2.49	0.43
1:A:286:LYS:HB3	1:A:286:LYS:HE2	1.55	0.43
1:A:303:ASN:CG	5:A:3014:HOH:O	2.56	0.43
1:C:129:ALA:HA	1:C:146:LEU:HD11	2.00	0.43
1:C:156:VAL:HG13	1:C:177:VAL:CG1	2.48	0.43
1:D:87:HIS:H	1:D:87:HIS:CD2	2.37	0.43
1:C:93:ILE:HG23	1:C:98:ILE:HB	2.01	0.43
1:C:274:GLU:HG2	1:D:138:TRP:CH2	2.54	0.43
1:C:106:VAL:CG1	1:C:304:THR:CG2	2.96	0.43
1:A:85:ILE:HG13	1:A:88:LEU:HD12	2.00	0.42
1:B:77:VAL:CG1	1:B:317:LEU:HD13	2.48	0.42
1:A:120:LEU:HG	1:B:117:SER:OG	2.18	0.42
1:A:59:LEU:HD21	4:A:3001:DGY:H3C2	2.00	0.42
1:C:114:LEU:O	1:C:114:LEU:HG	2.12	0.42
1:B:327:LYS:HD3	1:B:327:LYS:HA	1.62	0.42
1:C:263:ILE:O	5:C:3129:HOH:O	2.22	0.42
1:C:240:PHE:O	1:C:267:GLY:HA3	2.20	0.42
1:C:77:VAL:HG12	1:C:317:LEU:HD13	2.00	0.42
1:C:152:THR:HG23	1:C:152:THR:O	2.19	0.42
1:D:158:ILE:O	1:D:182:TYR:HA	2.19	0.42
1:D:109:ASP:CG	1:D:171:ARG:HH22	2.23	0.42
1:B:240:PHE:O	1:B:266:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:227:ASN:O	1:C:231:PHE:CD2	2.73	0.42
1:C:19:GLY:HA3	1:C:306:SER:OG	2.20	0.42
1:C:85:ILE:HG21	1:C:326:LEU:HD22	2.02	0.42
1:D:65:LYS:H	1:D:68:LEU:HD12	1.84	0.42
1:B:212:ILE:HD12	1:B:234:MET:HE3	2.00	0.42
1:A:16:PRO:HD3	1:B:143:PRO:HB2	2.02	0.42
1:C:235:LYS:C	1:C:237:THR:N	2.74	0.41
1:A:232:GLN:NE2	5:A:3087:HOH:O	2.53	0.41
1:C:131:GLU:OE2	1:C:135:ASN:ND2	2.53	0.41
1:D:281:PRO:HD3	5:D:2047:HOH:O	2.20	0.41
1:D:63:VAL:CG1	1:D:88:LEU:HD22	2.51	0.41
1:B:111:THR:CG2	3:B:2002:NDP:H41N	2.50	0.41
1:A:45:LEU:HD23	1:A:67:ILE:HG21	2.03	0.41
1:C:292:PRO:HD2	1:D:129:ALA:HB1	2.01	0.41
1:A:192:ALA:HB1	1:A:197:ALA:HB3	2.03	0.41
1:D:219:THR:HB	1:D:220:PRO:HD2	2.03	0.41
1:A:99:ARG:CD	1:A:325:GLU:OE1	2.68	0.41
1:A:114:LEU:HD22	1:A:295:GLY:HA2	2.03	0.41
1:C:182:TYR:CZ	1:C:199:PHE:HB2	2.54	0.41
1:A:277:PRO:C	1:A:279:ASN:H	2.25	0.41
1:B:269:ASP:O	1:B:293:HIS:HA	2.21	0.41
1:B:19:GLY:O	1:B:23:LEU:HG	2.20	0.41
1:D:8:LYS:NZ	1:D:52:ALA:HB2	2.36	0.40
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.85	0.40
1:A:216:CYS:HA	3:A:2001:NDP:O4B	2.20	0.40
1:B:118:LEU:HD22	1:B:267:GLY:HA3	2.03	0.40
1:A:56:LEU:HD23	1:A:57:CYS:N	2.36	0.40
1:D:240:PHE:O	1:D:266:ALA:HA	2.22	0.40
1:B:118:LEU:HG	1:B:291:LEU:HD12	2.02	0.40
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.91	0.40
1:C:126:LEU:N	1:C:127:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:14:ARG:NH2	1:C:96:ARG:O[1_655]	2.12	0.08

## 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	322/330 (98%)	311 (97%)	11 (3%)	0	100	100
1	B	321/330 (97%)	310 (97%)	10 (3%)	1 (0%)	50	53
1	C	322/330 (98%)	310 (96%)	10 (3%)	2 (1%)	33	32
1	D	321/330 (97%)	299 (93%)	16 (5%)	6 (2%)	12	7
All	All	1286/1320 (97%)	1230 (96%)	47 (4%)	9 (1%)	30	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	65	LYS
1	D	89	ALA
1	D	244	SER
1	B	244	SER
1	D	75	LEU
1	D	86	ASP
1	D	313	LEU
1	C	244	SER
1	C	295	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	265/270 (98%)	240 (91%)	25 (9%)	13	11
1	B	264/270 (98%)	239 (90%)	25 (10%)	12	11
1	C	265/270 (98%)	242 (91%)	23 (9%)	15	14
1	D	264/270 (98%)	231 (88%)	33 (12%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1058/1080 (98%)	952 (90%)	106 (10%)	11	10

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	LEU
1	A	32	GLU
1	A	43	LYS
1	A	47	ARG
1	A	55	LEU
1	A	66	ARG
1	A	67	ILE
1	A	85	ILE
1	A	90	LEU
1	A	102	TYR
1	A	107	LEU
1	A	120	LEU
1	A	151	LEU
1	A	172	LEU
1	A	179	ARG
1	A	183	THR
1	A	185	ARG
1	A	223	GLU
1	A	229	ASP
1	A	232	GLN
1	A	276	LEU
1	A	283	LEU
1	A	317	LEU
1	A	327	LYS
1	B	75	LEU
1	B	91	ASP
1	B	94	LYS
1	B	102	TYR
1	B	107	LEU
1	B	118	LEU
1	B	119	LEU
1	B	121	THR
1	B	131	GLU
1	B	153	GLN
1	B	172	LEU
1	B	190	GLU

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Mol	Chain	Res	Type
1	B	202	THR
1	B	204	GLU
1	B	205	LEU
1	B	208	GLN
1	B	228	LYS
1	B	229	ASP
1	B	252	ASP
1	B	254	LEU
1	B	276	LEU
1	B	279	ASN
1	B	308	LEU
1	B	317	LEU
1	B	326	LEU
1	C	20	ARG
1	C	76	LYS
1	C	83	VAL
1	C	102	TYR
1	C	107	LEU
1	C	108	THR
1	C	119	LEU
1	C	120	LEU
1	C	121	THR
1	C	131	GLU
1	C	145	TRP
1	C	153	GLN
1	C	156	VAL
1	C	172	LEU
1	C	183	THR
1	C	185	ARG
1	C	191	GLU
1	C	232	GLN
1	C	272	SER
1	C	276	LEU
1	C	308	LEU
1	C	317	LEU
1	C	327	LYS
1	D	7	MET
1	D	20	ARG
1	D	40	ILE
1	D	58	LEU
1	D	60	SER
1	D	67	ILE

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Mol	Chain	Res	Type
1	D	74	ASN
1	D	92	GLU
1	D	99	ARG
1	D	102	TYR
1	D	105	ASP
1	D	107	LEU
1	D	118	LEU
1	D	119	LEU
1	D	120	LEU
1	D	131	GLU
1	D	133	VAL
1	D	151	LEU
1	D	163	ARG
1	D	179	ARG
1	D	183	THR
1	D	186	GLN
1	D	195	PHE
1	D	217	SER
1	D	252	ASP
1	D	256	GLN
1	D	262	LYS
1	D	276	LEU
1	D	286	LYS
1	D	306	SER
1	D	308	LEU
1	D	326	LEU
1	D	327	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	280	HIS
1	B	53	HIS
1	B	178	GLN
1	B	208	GLN
1	B	279	ASN
1	B	280	HIS
1	B	299	HIS
1	C	53	HIS
1	C	62	HIS
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	153	GLN
1	C	178	GLN
1	C	196	GLN
1	C	232	GLN
1	C	280	HIS
1	D	53	HIS
1	D	186	GLN
1	D	280	HIS

### 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 ⓘ

11 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	$\# Z  > 2$
3	NDP	A	2001	-	52,52,52	1.43	5 (9%)	80,80,80	1.76	8 (10%)
4	DGY	A	3001	-	6,6,6	1.45	1 (16%)	7,7,7	1.21	0
2	SO4	B	1005	-	4,4,4	0.18	0	6,6,6	0.28	0
3	NDP	B	2002	-	52,52,52	1.47	5 (9%)	80,80,80	2.79	16 (20%)
2	SO4	C	1001	-	4,4,4	0.23	0	6,6,6	0.14	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDP	C	2003	-	52,52,52	1.37	5 (9%)	80,80,80	2.15	15 (18%)
4	DGY	C	3002	-	6,6,6	1.52	1 (16%)	7,7,7	1.16	0
2	SO4	D	1002	-	4,4,4	0.11	0	6,6,6	0.23	0
2	SO4	D	1003	-	4,4,4	0.09	0	6,6,6	0.36	0
2	SO4	D	1004	-	4,4,4	0.20	0	6,6,6	0.34	0
3	NDP	D	2004	-	52,52,52	1.44	6 (11%)	80,80,80	2.13	11 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	A	2001	-	-	0/35/77/77	0/3/5/5
4	DGY	A	3001	-	-	0/6/6/6	0/0/0/0
2	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
3	NDP	B	2002	-	-	0/35/77/77	0/3/5/5
2	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
3	NDP	C	2003	-	-	0/35/77/77	0/3/5/5
4	DGY	C	3002	-	-	0/6/6/6	0/0/0/0
2	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1004	-	-	0/0/0/0	0/0/0/0
3	NDP	D	2004	-	-	0/35/77/77	0/3/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	NDP	O7N-C7N	6.95	1.42	1.24
3	D	2004	NDP	O7N-C7N	6.51	1.41	1.24
3	A	2001	NDP	O7N-C7N	6.43	1.41	1.24
3	C	2003	NDP	O7N-C7N	5.89	1.39	1.24
3	B	2002	NDP	C2N-C3N	3.83	1.42	1.34
3	A	2001	NDP	C2A-N3A	3.64	1.39	1.32
3	D	2004	NDP	C2A-N3A	3.39	1.38	1.32
3	C	2003	NDP	C2A-N3A	3.23	1.38	1.32
3	D	2004	NDP	C2N-C3N	3.19	1.41	1.34
3	C	2003	NDP	C2N-C3N	3.13	1.40	1.34
3	C	2003	NDP	C6N-C5N	2.94	1.39	1.33
3	B	2002	NDP	C2A-N3A	2.93	1.38	1.32
3	A	2001	NDP	C6N-C5N	2.92	1.39	1.33
3	B	2002	NDP	C2A-N1A	2.83	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	DGY	C3-C2	2.71	1.55	1.51
3	A	2001	NDP	C2A-N1A	2.69	1.39	1.33
3	A	2001	NDP	C2N-C3N	2.64	1.39	1.34
3	C	2003	NDP	C2A-N1A	2.64	1.39	1.33
4	C	3002	DGY	C3-C2	2.55	1.55	1.51
3	D	2004	NDP	C6N-C5N	2.53	1.38	1.33
3	D	2004	NDP	C2A-N1A	2.40	1.38	1.33
3	B	2002	NDP	C6N-C5N	2.33	1.38	1.33
3	D	2004	NDP	PN-O3	2.27	1.64	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	NDP	O4B-C1B-N9A	14.52	121.94	108.44
3	B	2002	NDP	N3A-C2A-N1A	-12.35	118.38	128.71
3	D	2004	NDP	O4B-C1B-N9A	10.68	118.38	108.44
3	D	2004	NDP	N3A-C2A-N1A	-10.67	119.79	128.71
3	C	2003	NDP	N3A-C2A-N1A	-10.20	120.18	128.71
3	A	2001	NDP	N3A-C2A-N1A	-9.76	120.55	128.71
3	B	2002	NDP	C4B-O4B-C1B	-9.44	99.50	109.75
3	C	2003	NDP	O4B-C1B-N9A	8.92	116.73	108.44
3	C	2003	NDP	C4B-O4B-C1B	-7.26	101.86	109.75
3	A	2001	NDP	O4B-C1B-N9A	6.73	114.70	108.44
3	B	2002	NDP	O7N-C7N-C3N	-4.44	112.17	120.51
3	A	2001	NDP	N3A-C4A-N9A	3.80	132.30	125.43
3	D	2004	NDP	N3A-C4A-N9A	3.68	132.08	125.43
3	A	2001	NDP	O4B-C1B-C2B	-3.57	103.61	106.95
3	C	2003	NDP	O7N-C7N-C3N	-3.52	113.91	120.51
3	D	2004	NDP	PN-O3-PA	-3.37	121.81	131.68
3	A	2001	NDP	PN-O3-PA	-3.28	122.06	131.68
3	C	2003	NDP	C1B-N9A-C4A	-3.27	120.99	126.64
3	C	2003	NDP	N3A-C4A-N9A	3.20	131.22	125.43
3	B	2002	NDP	N3A-C4A-N9A	3.19	131.19	125.43
3	D	2004	NDP	C4B-O4B-C1B	-3.18	106.30	109.75
3	B	2002	NDP	C1B-N9A-C4A	-3.12	121.25	126.64
3	B	2002	NDP	O3B-C3B-C4B	-2.91	102.51	111.08
3	D	2004	NDP	O4B-C1B-C2B	-2.85	104.29	106.95
3	B	2002	NDP	O4B-C4B-C5B	2.83	119.45	109.36
3	B	2002	NDP	C3B-C2B-C1B	-2.80	97.29	102.73
3	B	2002	NDP	C3N-C2N-N1N	-2.78	119.10	123.05
3	C	2003	NDP	C4A-C5A-N7A	-2.74	107.17	109.52
3	D	2004	NDP	C5A-C4A-N3A	-2.70	119.81	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	NDP	C3N-C7N-N7N	2.68	122.63	117.48
3	C	2003	NDP	N7A-C8A-N9A	-2.54	107.17	114.36
3	B	2002	NDP	C2A-N3A-C4A	2.52	121.19	114.01
3	D	2004	NDP	C4A-C5A-N7A	-2.48	107.40	109.52
3	D	2004	NDP	C2A-N3A-C4A	2.45	120.99	114.01
3	D	2004	NDP	O7N-C7N-C3N	-2.43	115.95	120.51
3	C	2003	NDP	C8A-N9A-C4A	2.36	108.70	106.90
3	B	2002	NDP	C4A-C5A-N7A	-2.31	107.54	109.52
3	C	2003	NDP	C2D-C1D-N1N	-2.30	107.35	113.21
3	A	2001	NDP	C5A-C4A-N3A	-2.27	120.76	125.70
3	D	2004	NDP	O2X-P2B-O2B	2.24	113.55	107.09
3	C	2003	NDP	O4B-C1B-C2B	-2.24	104.86	106.95
3	B	2002	NDP	N7A-C8A-N9A	-2.21	108.12	114.36
3	B	2002	NDP	O5B-C5B-C4B	2.16	116.88	108.94
3	A	2001	NDP	N7A-C8A-N9A	-2.16	108.25	114.36
3	C	2003	NDP	C3N-C2N-N1N	-2.11	120.06	123.05
3	B	2002	NDP	C8A-N9A-C1B	2.09	130.50	126.38
3	A	2001	NDP	C2A-N3A-C4A	2.08	119.93	114.01
3	C	2003	NDP	C2A-N3A-C4A	2.07	119.89	114.01
3	C	2003	NDP	C5A-C4A-N3A	-2.02	121.30	125.70
3	B	2002	NDP	C3N-C7N-N7N	2.01	121.34	117.48

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	324/330 (98%)	0.36	15 (4%) 31 31	19, 31, 39, 56	9 (2%)
1	B	323/330 (97%)	0.09	3 (0%) 81 82	16, 28, 36, 49	12 (3%)
1	C	324/330 (98%)	0.35	16 (4%) 28 28	19, 32, 43, 50	21 (6%)
1	D	323/330 (97%)	0.85	46 (14%) 3 3	19, 34, 54, 65	42 (13%)
All	All	1294/1320 (98%)	0.41	80 (6%) 19 19	16, 31, 47, 65	84 (6%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	ALA	12.3
1	D	65	LYS	5.4
1	D	49	VAL	4.6
1	D	51	GLY	4.5
1	A	27	ALA	4.2
1	A	6	LEU	4.2
1	C	185	ARG	4.1
1	D	72	GLY	4.1
1	D	50	ALA	4.0
1	D	89	ALA	3.8
1	D	90	LEU	3.7
1	C	116	VAL	3.6
1	D	48	GLY	3.6
1	C	199	PHE	3.6
1	D	78	ILE	3.4
1	A	220	PRO	3.4
1	D	73	ALA	3.3
1	D	64	ASP	3.2
1	D	88	LEU	3.1
1	D	67	ILE	3.1
1	A	5	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	75	LEU	3.0
1	D	86	ASP	3.0
1	D	34	TRP	3.0
1	D	45	LEU	3.0
1	D	63	VAL	2.9
1	D	316	GLY	2.9
1	D	327	LYS	2.9
1	C	189	PRO	2.9
1	D	321	PRO	2.8
1	D	220	PRO	2.8
1	A	28	ASP	2.8
1	D	69	ASP	2.8
1	D	317	LEU	2.7
1	C	197	ALA	2.7
1	C	188	ARG	2.7
1	D	98	ILE	2.7
1	A	328	LEU	2.6
1	D	40	ILE	2.6
1	D	29	CYS	2.6
1	A	206	ALA	2.6
1	C	117	SER	2.6
1	D	6	LEU	2.6
1	D	54	GLY	2.5
1	D	93	ILE	2.5
1	A	31	VAL	2.5
1	B	91	ASP	2.5
1	C	193	ALA	2.5
1	D	7	MET	2.5
1	A	321	PRO	2.5
1	C	186	GLN	2.5
1	C	196	GLN	2.5
1	D	66	ARG	2.5
1	A	24	ALA	2.5
1	D	70	ALA	2.5
1	D	308	LEU	2.4
1	D	315	ALA	2.4
1	C	120	LEU	2.4
1	D	116	VAL	2.4
1	B	315	ALA	2.3
1	A	25	ARG	2.3
1	A	185	ARG	2.3
1	A	221	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	100	VAL	2.3
1	D	44	GLU	2.2
1	D	119	LEU	2.2
1	C	121	THR	2.2
1	C	192	ALA	2.2
1	D	309	ALA	2.2
1	B	220	PRO	2.2
1	C	205	LEU	2.2
1	C	232	GLN	2.1
1	D	221	ALA	2.1
1	D	222	THR	2.1
1	C	266	ALA	2.1
1	D	99	ARG	2.0
1	A	23	LEU	2.0
1	A	313	LEU	2.0
1	D	91	ASP	2.0
1	D	328	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	C	1001	5/5	0.32	6.30	110,110,110,111	0
3	NDP	B	2002	48/48	0.33	6.01	17,30,40,42	48
3	NDP	D	2004	48/48	0.37	4.66	30,48,50,52	48
2	SO4	D	1002	5/5	0.17	3.22	86,87,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	1003	5/5	0.19	3.06	72,72,73,74	0
4	DGY	C	3002	7/7	0.18	2.80	44,47,48,49	0
4	DGY	A	3001	7/7	0.18	1.44	38,40,43,44	0
3	NDP	A	2001	48/48	0.21	0.76	31,53,58,59	48
3	NDP	C	2003	48/48	0.20	0.29	28,54,63,64	48
2	SO4	B	1005	5/5	0.16	0.28	78,79,80,80	0
2	SO4	D	1004	5/5	0.15	-0.19	85,85,85,86	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.