



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:56 AM UTC

PDB ID : 2GCG / pdb_00002gcg
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

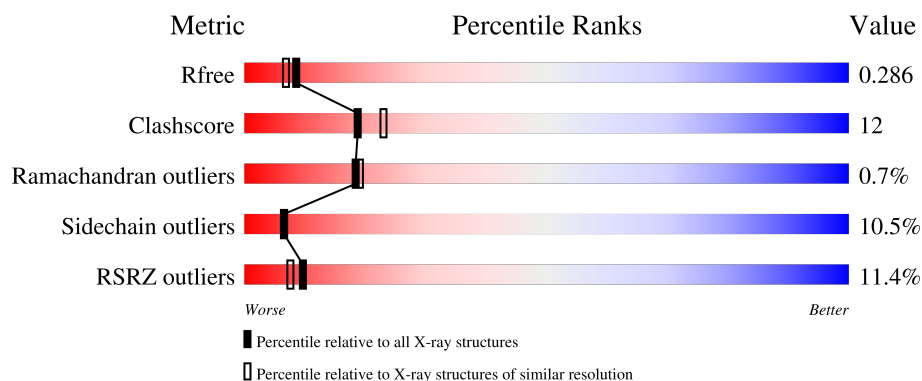
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

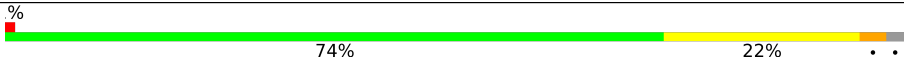
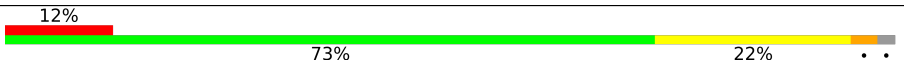
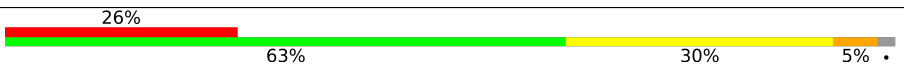
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	330	
1	B	330	
1	C	330	
1	D	330	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DGY	A	3001	-	-	X	-
3	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 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.

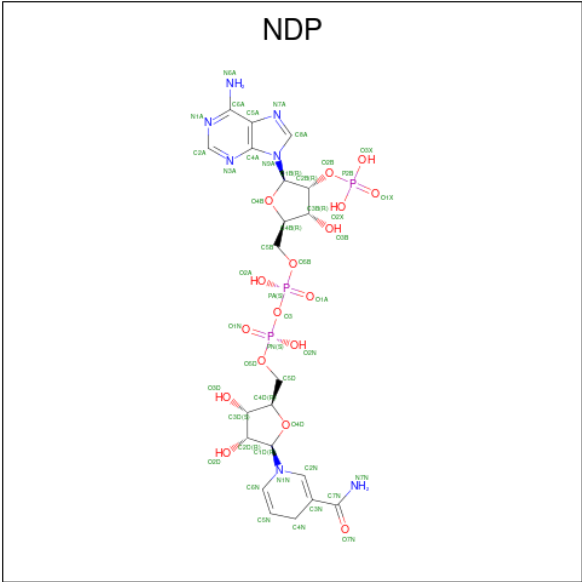
- Molecule 1 is a protein called Glyoxylate reductase/hydroxypyruvate reductase.

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:

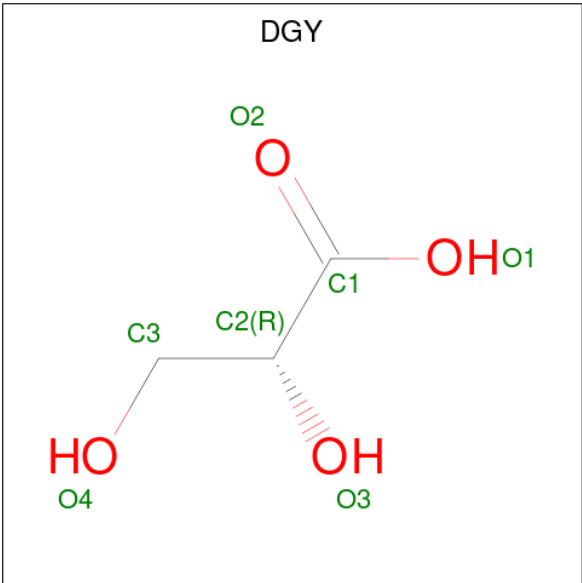
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	cloning artifact	UNP Q9UBQ7
A	0	SER	-	cloning artifact	UNP Q9UBQ7
B	-1	ALA	-	cloning artifact	UNP Q9UBQ7
B	0	SER	-	cloning artifact	UNP Q9UBQ7
C	-1	ALA	-	cloning artifact	UNP Q9UBQ7
C	0	SER	-	cloning artifact	UNP Q9UBQ7
D	-1	ALA	-	cloning artifact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

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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 (2R)-2,3-DIHYDROXYPROPANOIC ACID (CCD ID: DGY) (formula: C₃H₆O₄).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

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

Continued on next page...

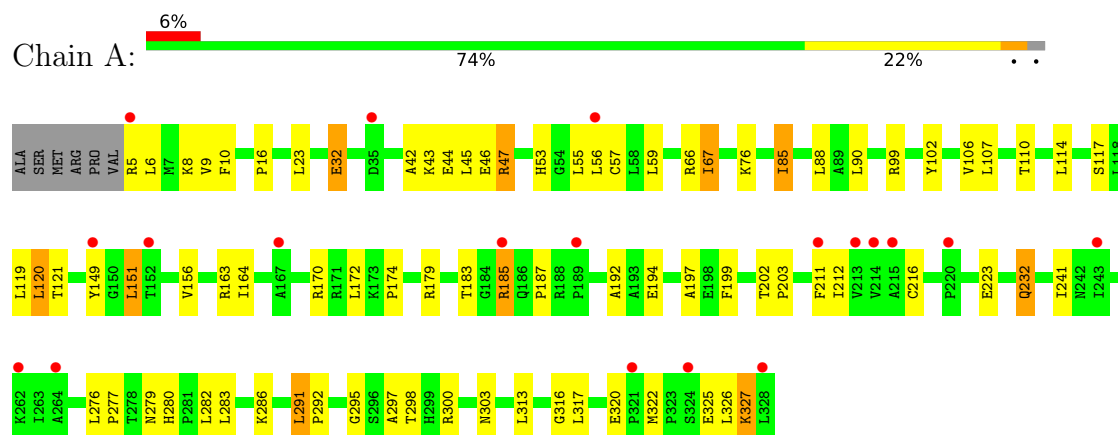
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	129	Total 129	O 129	0	0

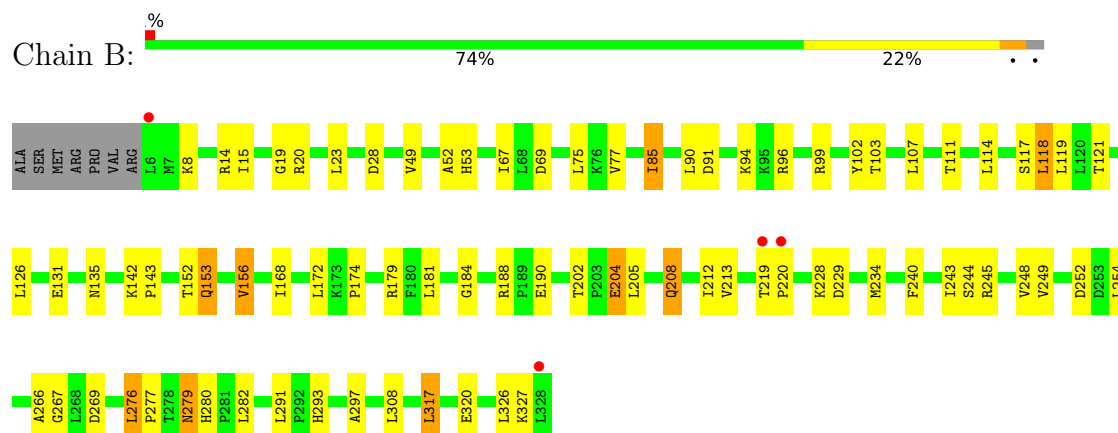
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

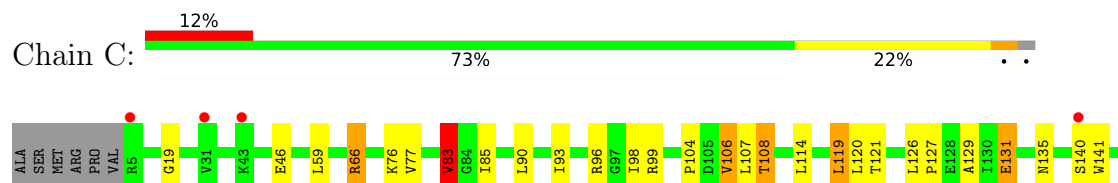
- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

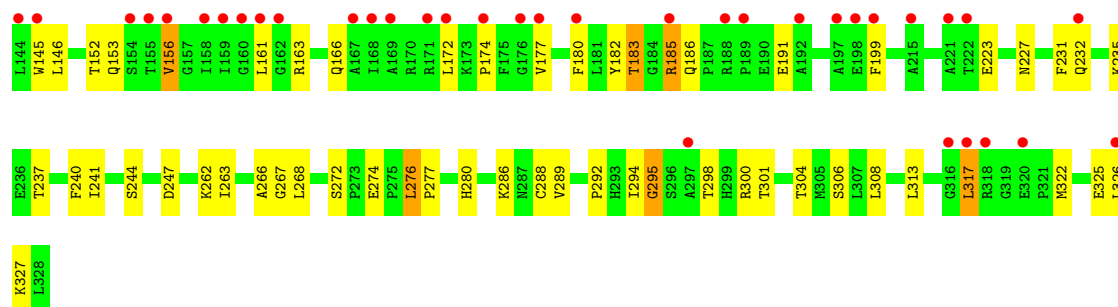


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase

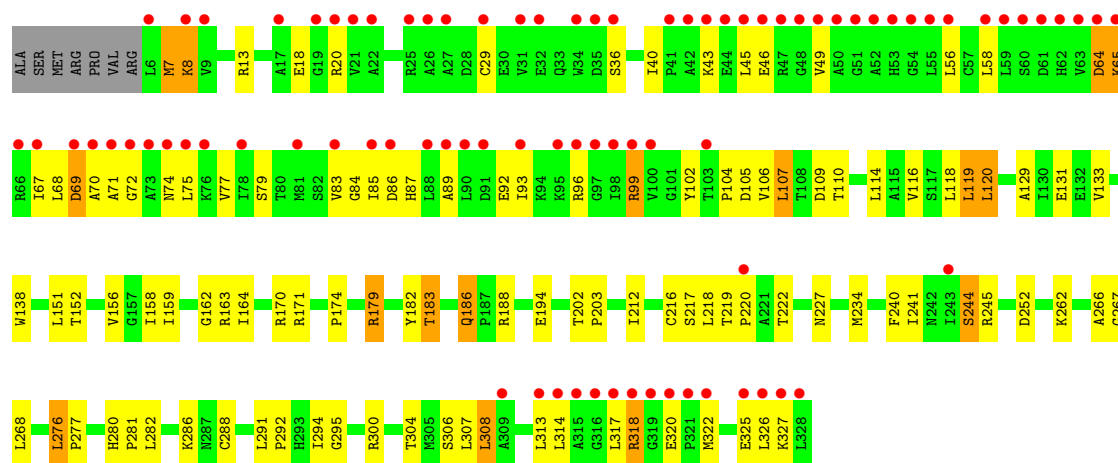


- Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase





● Molecule 1: Glyoxylate reductase/hydroxypyruvate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.57Å 66.88Å 149.78Å 90.00° 98.22° 90.00°	Depositor
Resolution (Å)	46.20 – 2.20 46.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.0 (46.20-2.20) 90.2 (46.20-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.201 , 0.282 0.208 , 0.286	Depositor DCC
R_{free} test set	3460 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10701	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGY, SO4, 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	1.01	0/2515	1.14	5/3414 (0.1%)
1	B	1.06	2/2503 (0.1%)	1.17	5/3400 (0.1%)
1	C	0.98	2/2514 (0.1%)	1.13	4/3414 (0.1%)
1	D	1.00	4/2503 (0.2%)	1.15	6/3400 (0.2%)
All	All	1.01	8/10035 (0.1%)	1.15	20/13628 (0.1%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	ASP	CG-OD1	10.06	1.44	1.25
1	D	69	ASP	CG-OD2	8.43	1.41	1.25
1	D	8	LYS	CE-NZ	6.66	1.69	1.49
1	C	298	THR	CA-C	-6.45	1.44	1.52
1	B	168	ILE	CA-CB	6.13	1.61	1.54
1	B	156	VAL	CA-CB	5.92	1.61	1.54
1	D	318	ARG	CZ-NH2	5.18	1.40	1.33
1	C	106	VAL	CA-CB	5.03	1.60	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	268	LEU	N-CA-C	9.53	124.43	108.90
1	A	291	LEU	CA-C-N	8.27	133.08	121.91
1	A	291	LEU	C-N-CA	8.27	133.08	121.91
1	C	298	THR	N-CA-C	-7.70	97.59	109.52
1	C	83	VAL	CB-CA-C	-7.69	102.25	111.94
1	D	110	THR	N-CA-C	7.58	119.19	111.07
1	B	142	LYS	CA-C-N	7.16	127.16	119.28
1	B	142	LYS	C-N-CA	7.16	127.16	119.28
1	A	298	THR	N-CA-C	-5.92	100.06	109.23
1	C	301	THR	N-CA-C	5.63	117.09	111.07
1	C	268	LEU	N-CA-C	5.62	118.06	108.90
1	A	110	THR	N-CA-C	5.54	118.04	111.33
1	D	119	LEU	CA-CB-CG	5.37	135.10	116.30
1	B	103	THR	CA-C-N	5.30	125.28	120.03
1	B	103	THR	C-N-CA	5.30	125.28	120.03
1	A	297	ALA	N-CA-C	5.28	117.91	107.98
1	B	249	VAL	N-CA-C	5.26	116.16	108.58
1	D	291	LEU	CA-C-N	5.20	126.34	119.84
1	D	291	LEU	C-N-CA	5.20	126.34	119.84
1	D	179	ARG	N-CA-C	5.02	116.68	108.55

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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2471	0	2528	59	0
1	B	2459	0	2515	43	1
1	C	2470	0	2528	65	1
1	D	2459	0	2515	79	0
2	A	48	0	26	10	0
2	B	48	0	26	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	26	4	0
2	D	48	0	26	7	0
3	A	7	0	5	7	0
3	C	7	0	5	4	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	15	0	0	0	0
5	A	168	0	0	7	0
5	B	182	0	0	2	0
5	C	132	0	0	6	0
5	D	129	0	0	2	0
All	All	10701	0	10200	241	1

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 12.

All (241) 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:D:114:LEU:HD11	1:D:294:ILE:HG13	1.31	1.08
2:C:2003:NDP:H42N	3:C:3002:DGY:H2	1.37	1.05
1:A:149:TYR:HD1	5:A:3166:HOH:O	1.43	1.00
1:B:212:ILE:HD12	1:B:234:MET:HE3	1.44	0.99
1:A:163:ARG:HG2	5:A:3010:HOH:O	1.62	0.98
2:A:2001:NDP:C4N	3:A:3001:DGY:H2	1.93	0.97
2:C:2003:NDP:C4N	3:C:3002:DGY:H2	1.99	0.93
2:A:2001:NDP:H42N	3:A:3001:DGY:H2	1.49	0.93
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:C:85:ILE:HD13	1:C:90:LEU:HD11	1.56	0.87
1:C:183:THR:HG22	2:C:2003:NDP:H2A	1.58	0.85
1:D:64:ASP:CA	1:D:65:LYS:HB2	2.06	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	2:D:2004:NDP:H51N	1.63	0.78
1:C:153:GLN:HE21	1:C:153:GLN:HA	1.48	0.78
2: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:B:69:ASP:OD2	1:B:96:ARG:NH2	2.21	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:O	1:D:318:ARG:HD2	1.88	0.73
1:D:77:VAL:HG21	1:D:322:MET:HE1	1.69	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: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:D:234:MET:HE1	1:D:240:PHE:HB2	1.72	0.70
1:C:108:THR:HG21	5:C:3006:HOH:O	1.90	0.70
2:D:2004:NDP:O1X	5:D:2107:HOH:O	2.10	0.69
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.04	0.69
1:A:164:ILE:HD12	2: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	3:A:3001:DGY:H3C2	2.26	0.66
1:B:8:LYS:H	1:B:53:HIS:HD2	1.43	0.65
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: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	2:D:2004:NDP:O3B	2.31	0.64
1:A:76:LYS:NZ	1:A:316:GLY:O	2.31	0.64
1:D:77:VAL:CG2	1:D:322:MET:HE1	2.28	0.63
1:D:162:GLY:HA3	2:D:2004:NDP:O1A	1.99	0.62
1:A:170:ARG:HD3	1:A:194:GLU:OE2	1.99	0.62
1:D:114:LEU:CD1	1:D:294:ILE:O	2.47	0.62
1:A:300:ARG:HH12	1:B:153:GLN:HG2	1.62	0.61
2:A:2001:NDP:C5N	3:A:3001:DGY:H2	2.29	0.61
1:B:212:ILE:HD12	1:B:234:MET:CE	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	1:B:126:LEU:HD22	1.82	0.61
1:C:83:VAL:HG13	1:C:104:PRO:HA	1.80	0.61
1:C:276:LEU:CD2	1:C:277:PRO:HD2	2.31	0.61
2:A:2001:NDP:C3N	3: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	2:A:2001:NDP:O3X	2.01	0.60
1:D:83:VAL:HG11	2:D:2004:NDP:H6N	1.83	0.60
1:D:29:CYS:SG	1:D:317:LEU:CD2	2.90	0.60
2:C:2003:NDP:C3N	3: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:A:119:LEU:HD13	1:A:241:ILE:HG13	1.84	0.59
1:B:279:ASN:H	1:B:279:ASN:HD22	1.51	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:D:70:ALA:HA	1:D:71:ALA:C	2.29	0.58
1:C:140:SER:OG	1:C:141:TRP:N	2.35	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
1:C:153:GLN:HA	1:C:153:GLN:NE2	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
1:D:7:MET:HE2	1:D:317:LEU:HB3	1.89	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:D:212:ILE:HD12	1:D:234:MET:HE3	1.89	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:C:129:ALA:HB1	1:D:292:PRO:HD2	1.90	0.54
1:D:159:ILE:HA	1:D:183:THR:HG22	1.90	0.54
1:C:114:LEU:CD2	1:C:295:GLY:HA2	2.37	0.53
1:C:46:GLU:CD	1:C:66:ARG:HD3	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:HB3	1:C:322:MET:HE1	1.89	0.53
1:B:204:GLU:O	1:B:208:GLN:HG2	2.07	0.53
1:C:235:LYS:C	1:C:237:THR:H	2.16	0.52
1:B:49:VAL:O	1:B:49:VAL:HG22	2.08	0.52
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	2:A:2001:NDP:O2X	2.41	0.52
1:B:118:LEU:HG	1:B:291:LEU:CD1	2.40	0.52
1:D:114:LEU:HD13	1:D:294:ILE:C	2.35	0.52
1:C:77:VAL:CG1	1:C:317:LEU:HD13	2.40	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:A:291:LEU:HB3	1:A:292:PRO:HD2	1.92	0.51
1:C:185:ARG:HD2	1:C:186:GLN:HB3	1.92	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:114:LEU:C	1:D:114:LEU:HD23	2.36	0.50
1:B:114:LEU:O	1:B:114:LEU:HG	2.03	0.50
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
1:A:44:GLU:OE2	1:A:47:ARG:NH2	2.46	0.49
1:C:294:ILE:O	1:C:295:GLY:C	2.54	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	2:D:2004:NDP:O7N	2.13	0.49
1:B:276:LEU:HD22	1:B:277:PRO:HD2	1.94	0.48
1:A:8:LYS:H	1:A:53:HIS:HD2	1.62	0.48
1:A:121:THR:HG21	1:B:126:LEU:CD2	2.42	0.48
1:B:184:GLY:HA2	2:B:2002:NDP:C2A	2.43	0.48
1:C:114:LEU:HD22	1:C:295:GLY:CA	2.43	0.48
1:A:114:LEU:O	1:A:114:LEU:HG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HG3	1:B:52:ALA:HA	1.96	0.48
1:D:240:PHE:O	1:D:267:GLY:HA3	2.14	0.48
1:A:303:ASN:CG	5:A:3014:HOH:O	2.56	0.47
1:A:156:VAL:HG22	1:A:211:PHE:HB2	1.95	0.47
1:D:83:VAL:CG1	2:D:2004:NDP:H6N	2.44	0.47
1:A:322:MET:HB2	1:A:325:GLU:HB2	1.96	0.47
1:B:234:MET:HE1	1:B:240:PHE:HB2	1.96	0.47
1:D:109:ASP:CG	1:D:171:ARG:HH22	2.23	0.47
1:D:276:LEU:HD22	1:D:277:PRO:CD	2.44	0.47
1:C:59:LEU:CD2	3: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: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:262:LYS:NZ	5:C:3111:HOH:O	2.44	0.46
1:B:118:LEU:HG	1:B:291:LEU:HD11	1.99	0.45
1:A:327:LYS:NZ	1:A:327:LYS:HB3	2.30	0.45
1:D:186:GLN:HE21	1:D:186:GLN:HB3	1.56	0.45
1:A:277:PRO:C	1:A:279:ASN:H	2.25	0.45
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:C:223:GLU:HG3	1:C:247:ASP:HB3	1.99	0.45
1:D:83:VAL:HG13	1:D:84:GLY:N	2.31	0.45
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:A:277:PRO:C	1:A:279:ASN:N	2.76	0.44
1:C:235:LYS:C	1:C:237:THR:N	2.74	0.44
1:C:153:GLN:HB2	1:D:300:ARG:HH22	1.82	0.44
1:A:42:ALA:O	1:A:46:GLU:HG3	2.18	0.44
1:B:77:VAL:HG12	1:B:317:LEU:HD13	2.00	0.44
1:D:18:GLU:OE2	1:D:307:LEU:HD22	2.18	0.44
1:D:114:LEU:CD1	1:D:294:ILE:C	2.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2001:NDP:H42N	3:A:3001:DGY:C2	2.34	0.43
1:B:28:ASP:OD1	1:B:28:ASP:N	2.51	0.43
1:C:106:VAL:CG1	1:C:304:THR:HG22	2.47	0.43
1:C:266:ALA:HB1	1:C:267:GLY:HA3	1.99	0.43
1:C:129:ALA:HA	1:C:146:LEU:CD1	2.49	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:A:286:LYS:HE2	1:A:286:LYS:HB3	1.55	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:C:93:ILE:HG23	1:C:98:ILE:HB	2.01	0.43
1:D:87:HIS:H	1:D:87:HIS:CD2	2.37	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:D:227:ASN:OD1	1:D:227:ASN:C	2.62	0.43
1:A:85:ILE:HG13	1:A:88:LEU:HD12	2.00	0.42
1:A:120:LEU:HG	1:B:117:SER:OG	2.18	0.42
1:B:77:VAL:CG1	1:B:317:LEU:HD13	2.48	0.42
1:B:135:ASN:OD1	1:B:135:ASN:C	2.62	0.42
1:A:59:LEU:HD21	3:A:3001:DGY:H3C2	2.00	0.42
1:B:327:LYS:HA	1:B:327:LYS:HD3	1.62	0.42
1:C:114:LEU:O	1:C:114:LEU:HG	2.12	0.42
1:C:263:ILE:O	5:C:3129:HOH:O	2.22	0.42
1:A:56:LEU:C	1:A:56:LEU:HD23	2.44	0.42
1:C:77:VAL:HG12	1:C:317:LEU:HD13	2.00	0.42
1:C:240:PHE:O	1:C:267:GLY:HA3	2.20	0.42
1:B:240:PHE:O	1:B:266:ALA:HA	2.19	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: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:A:16:PRO:HD3	1:B:143:PRO:HB2	2.02	0.42
1:D:65:LYS:H	1:D:68:LEU:HD12	1.84	0.42
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:A:45:LEU:HD23	1:A:67:ILE:HG21	2.03	0.41
1:B:111:THR:CG2	2:B:2002:NDP:H41N	2.50	0.41
1:A:192:ALA:HB1	1:A:197:ALA:HB3	2.03	0.41
1:C:292:PRO:HD2	1:D:129:ALA:HB1	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:19:GLY:O	1:B:23:LEU:HG	2.20	0.41
1:B:269:ASP:O	1:B:293:HIS:HA	2.21	0.41
1:A:23:LEU:HA	1:A:23:LEU:HD23	1.85	0.40
1:A:216:CYS:HA	2:A:2001:NDP:O4B	2.20	0.40
1:A:56:LEU:HD23	1:A:57:CYS:N	2.36	0.40
1:B:118:LEU:HD22	1:B:267:GLY:HA3	2.03	0.40
1:B:118:LEU:HG	1:B:291:LEU:HD12	2.02	0.40
1:D:240:PHE:O	1:D:266:ALA:HA	2.22	0.40
1:D:308:LEU:HD23	1:D:308:LEU:HA	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	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:NH2	1:C:96:ARG:O[1_655]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/330 (98%)	311 (97%)	11 (3%)	0	100	100
1	B	321/330 (97%)	310 (97%)	10 (3%)	1 (0%)	36	42
1	C	322/330 (98%)	310 (96%)	10 (3%)	2 (1%)	21	23
1	D	321/330 (97%)	299 (93%)	16 (5%)	6 (2%)	6	4
All	All	1286/1320 (97%)	1230 (96%)	47 (4%)	9 (1%)	18	19

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%)	239 (90%)	26 (10%)	7	8
1	B	264/270 (98%)	234 (89%)	30 (11%)	5	5
1	C	265/270 (98%)	243 (92%)	22 (8%)	10	11
1	D	264/270 (98%)	231 (88%)	33 (12%)	4	4
All	All	1058/1080 (98%)	947 (90%)	111 (10%)	6	6

All (111) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	VAL
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	212	ILE
1	A	223	GLU
1	A	232	GLN
1	A	276	LEU
1	A	283	LEU
1	A	317	LEU
1	A	327	LYS
1	B	67	ILE
1	B	75	LEU
1	B	85	ILE
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	156	VAL
1	B	172	LEU
1	B	190	GLU
1	B	202	THR
1	B	204	GLU
1	B	205	LEU
1	B	208	GLN
1	B	213	VAL
1	B	228	LYS
1	B	229	ASP
1	B	243	ILE
1	B	252	ASP
1	B	254	LEU
1	B	276	LEU
1	B	279	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	308	LEU
1	B	317	LEU
1	B	326	LEU
1	C	66	ARG
1	C	76	LYS
1	C	83	VAL
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	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	286	LYS
1	C	308	LEU
1	C	313	LEU
1	C	317	LEU
1	C	327	LYS
1	D	7	MET
1	D	8	LYS
1	D	20	ARG
1	D	40	ILE
1	D	58	LEU
1	D	67	ILE
1	D	74	ASN
1	D	85	ILE
1	D	92	GLU
1	D	93	ILE
1	D	99	ARG
1	D	105	ASP
1	D	107	LEU
1	D	118	LEU
1	D	119	LEU
1	D	120	LEU
1	D	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	133	VAL
1	D	151	LEU
1	D	156	VAL
1	D	163	ARG
1	D	179	ARG
1	D	183	THR
1	D	186	GLN
1	D	217	SER
1	D	252	ASP
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	53	HIS
1	A	62	HIS
1	A	166	GLN
1	A	280	HIS
1	B	53	HIS
1	B	153	GLN
1	B	178	GLN
1	B	208	GLN
1	B	232	GLN
1	B	279	ASN
1	B	280	HIS
1	B	299	HIS
1	C	62	HIS
1	C	74	ASN
1	C	153	GLN
1	C	178	GLN
1	C	196	GLN
1	C	303	ASN
1	D	33	GLN
1	D	53	HIS
1	D	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	186	GLN
1	D	280	HIS
1	D	303	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	SO4	D	1004	-	4,4,4	0.29	0	6,6,6	0.32	0
2	NDP	B	2002	-	51,52,52	1.52	5 (9%)	71,80,80	2.13	20 (28%)
4	SO4	D	1002	-	4,4,4	0.26	0	6,6,6	0.36	0
2	NDP	D	2004	-	51,52,52	1.62	7 (13%)	71,80,80	1.79	13 (18%)
2	NDP	A	2001	-	51,52,52	1.55	7 (13%)	71,80,80	1.55	10 (14%)
4	SO4	D	1003	-	4,4,4	0.25	0	6,6,6	0.28	0
3	DGY	A	3001	-	6,6,6	1.54	1 (16%)	6,7,7	1.42	1 (16%)
4	SO4	B	1005	-	4,4,4	0.22	0	6,6,6	0.26	0
2	NDP	C	2003	-	51,52,52	1.46	8 (15%)	71,80,80	1.83	16 (22%)
4	SO4	C	1001	-	4,4,4	0.27	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DGY	C	3002	-	6,6,6	1.64	1 (16%)	6,7,7	1.49	1 (16%)

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	B	2002	-	-	7/34/77/77	0/5/5/5
2	NDP	D	2004	-	-	15/34/77/77	0/5/5/5
2	NDP	A	2001	-	-	11/34/77/77	0/5/5/5
3	DGY	A	3001	-	-	1/6/6/6	-
2	NDP	C	2003	-	-	9/34/77/77	0/5/5/5
3	DGY	C	3002	-	-	1/6/6/6	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	NDP	O7N-C7N	7.78	1.42	1.24
2	D	2004	NDP	O7N-C7N	7.29	1.41	1.24
2	A	2001	NDP	O7N-C7N	7.20	1.41	1.24
2	C	2003	NDP	O7N-C7N	6.60	1.39	1.24
2	D	2004	NDP	PN-O3	4.16	1.64	1.59
2	A	2001	NDP	PN-O3	3.33	1.63	1.59
2	B	2002	NDP	C2A-N1A	3.13	1.39	1.33
2	A	2001	NDP	C2A-N3A	3.07	1.39	1.33
2	A	2001	NDP	C2A-N1A	2.97	1.39	1.33
2	C	2003	NDP	C2A-N1A	2.91	1.39	1.33
2	D	2004	NDP	C2A-N3A	2.79	1.38	1.33
2	D	2004	NDP	PA-O3	2.67	1.62	1.59
3	A	3001	DGY	C3-C2	2.66	1.55	1.51
2	D	2004	NDP	C2A-N1A	2.65	1.38	1.33
2	C	2003	NDP	C2A-N3A	2.60	1.38	1.33
2	B	2002	NDP	C2N-C3N	2.57	1.42	1.35
2	D	2004	NDP	C8A-N7A	2.55	1.36	1.31
3	C	3002	DGY	C3-C2	2.49	1.55	1.51
2	C	2003	NDP	PN-O3	2.46	1.62	1.59
2	B	2002	NDP	C8A-N7A	2.32	1.36	1.31
2	B	2002	NDP	C2A-N3A	2.27	1.38	1.33
2	C	2003	NDP	PA-O3	2.26	1.61	1.59
2	C	2003	NDP	C8A-N7A	2.25	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	NDP	PA-O3	2.17	1.61	1.59
2	D	2004	NDP	C2N-C3N	2.11	1.41	1.35
2	C	2003	NDP	C6N-C5N	2.10	1.39	1.33
2	A	2001	NDP	C6N-C5N	2.09	1.39	1.33
2	C	2003	NDP	C2N-C3N	2.07	1.40	1.35
2	A	2001	NDP	C8A-N7A	2.00	1.35	1.31

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	NDP	O4B-C1B-N9A	7.21	121.94	108.09
2	B	2002	NDP	N3A-C2A-N1A	-6.74	118.38	128.58
2	D	2004	NDP	N3A-C2A-N1A	-5.81	119.79	128.58
2	C	2003	NDP	N3A-C2A-N1A	-5.55	120.18	128.58
2	D	2004	NDP	O4B-C1B-N9A	5.36	118.38	108.09
2	A	2001	NDP	N3A-C2A-N1A	-5.31	120.55	128.58
2	D	2004	NDP	C5A-C4A-N3A	-5.01	119.81	126.72
2	C	2003	NDP	N9A-C8A-N7A	-4.77	107.17	113.94
2	B	2002	NDP	O7N-C7N-C3N	-4.63	112.17	120.90
2	B	2002	NDP	C4B-O4B-C1B	-4.51	99.50	109.47
2	C	2003	NDP	O4B-C1B-N9A	4.50	116.73	108.09
2	A	2001	NDP	C5A-C4A-N3A	-4.33	120.76	126.72
2	B	2002	NDP	N9A-C8A-N7A	-4.10	108.12	113.94
2	A	2001	NDP	N9A-C8A-N7A	-4.01	108.25	113.94
2	C	2003	NDP	C5A-C4A-N3A	-3.93	121.30	126.72
2	B	2002	NDP	C5A-C4A-N3A	-3.85	121.41	126.72
2	B	2002	NDP	C2A-N3A-C4A	3.83	121.19	111.83
2	C	2003	NDP	C5A-N7A-C8A	3.83	109.47	103.45
2	D	2004	NDP	C2A-N3A-C4A	3.75	120.99	111.83
2	C	2003	NDP	O7N-C7N-C3N	-3.71	113.91	120.90
2	C	2003	NDP	C4B-O4B-C1B	-3.44	101.86	109.47
2	A	2001	NDP	O4B-C1B-N9A	3.44	114.70	108.09
2	D	2004	NDP	C5A-N7A-C8A	3.39	108.78	103.45
2	D	2004	NDP	N9A-C8A-N7A	-3.38	109.14	113.94
2	A	2001	NDP	C5A-N7A-C8A	3.37	108.74	103.45
2	B	2002	NDP	C5A-N7A-C8A	3.34	108.71	103.45
2	A	2001	NDP	C2A-N3A-C4A	3.32	119.93	111.83
2	C	2003	NDP	C2A-N3A-C4A	3.30	119.89	111.83
2	B	2002	NDP	O4B-C4B-C5B	3.16	119.45	109.33
2	A	2001	NDP	N3A-C4A-N9A	3.02	132.30	127.17
2	B	2002	NDP	O3B-C3B-C4B	-2.99	102.51	111.08
2	C	2003	NDP	C4A-C5A-N7A	-2.98	107.17	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2004	NDP	N3A-C4A-N9A	2.89	132.08	127.17
2	B	2002	NDP	C3B-C2B-C1B	-2.88	97.29	102.81
2	C	2003	NDP	C4A-N9A-C8A	2.82	108.70	105.74
2	B	2002	NDP	C3N-C2N-N1N	-2.80	119.10	123.20
2	C	2003	NDP	C3N-C7N-N7N	2.79	122.63	117.67
2	D	2004	NDP	C4A-C5A-N7A	-2.79	107.40	110.58
2	D	2004	NDP	C2B-C1B-N9A	-2.69	109.32	113.75
2	B	2002	NDP	C4A-C5A-N7A	-2.66	107.54	110.58
2	D	2004	NDP	O7N-C7N-C3N	-2.63	115.95	120.90
2	C	2003	NDP	C2D-C1D-N1N	-2.42	107.35	113.31
2	C	2003	NDP	C4A-N9A-C1B	-2.41	120.99	126.63
3	C	3002	DGY	O2-C1-C2	-2.40	117.80	122.60
2	C	2003	NDP	N3A-C4A-N9A	2.38	131.22	127.17
2	B	2002	NDP	C4A-N9A-C8A	2.37	108.23	105.74
2	B	2002	NDP	N3A-C4A-N9A	2.36	131.19	127.17
2	B	2002	NDP	O5B-C5B-C4B	2.32	116.88	108.99
2	B	2002	NDP	C4A-N9A-C1B	-2.30	121.25	126.63
2	D	2004	NDP	C6A-C5A-C4A	2.25	120.25	117.18
2	A	2001	NDP	C4A-C5A-N7A	-2.23	108.03	110.58
3	A	3001	DGY	O2-C1-C2	-2.22	118.17	122.60
2	A	2001	NDP	C4A-N9A-C8A	2.19	108.04	105.74
2	D	2004	NDP	O2A-PA-O3	2.16	113.10	107.27
2	C	2003	NDP	C3N-C2N-N1N	-2.14	120.06	123.20
2	C	2003	NDP	C6N-N1N-C2N	2.11	121.58	119.32
2	D	2004	NDP	C5A-C4A-N9A	2.09	108.09	105.81
2	B	2002	NDP	O2N-PN-O1N	2.09	122.17	112.44
2	A	2001	NDP	C1D-N1N-C2N	-2.08	117.72	121.14
2	B	2002	NDP	C3N-C7N-N7N	2.07	121.34	117.67
2	B	2002	NDP	C1D-N1N-C6N	-2.06	116.42	120.77

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	NDP	C5B-O5B-PA-O1A
2	A	2001	NDP	C5B-O5B-PA-O2A
2	A	2001	NDP	C5B-O5B-PA-O3
2	A	2001	NDP	C5D-O5D-PN-O2N
2	D	2004	NDP	C5D-O5D-PN-O3
2	D	2004	NDP	C5D-O5D-PN-O1N
2	D	2004	NDP	C5D-O5D-PN-O2N
3	C	3002	DGY	O3-C2-C3-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	2004	NDP	O4B-C4B-C5B-O5B
2	D	2004	NDP	C3B-C4B-C5B-O5B
2	D	2004	NDP	O4D-C4D-C5D-O5D
2	D	2004	NDP	C3D-C4D-C5D-O5D
2	D	2004	NDP	C1B-C2B-O2B-P2B
2	C	2003	NDP	O4B-C4B-C5B-O5B
2	C	2003	NDP	C3B-C4B-C5B-O5B
2	C	2003	NDP	O4D-C4D-C5D-O5D
2	B	2002	NDP	C2N-C3N-C7N-N7N
2	A	2001	NDP	PN-O3-PA-O5B
2	A	2001	NDP	O4D-C4D-C5D-O5D
2	D	2004	NDP	C3B-C2B-O2B-P2B
3	A	3001	DGY	O3-C2-C3-O4
2	B	2002	NDP	O4D-C1D-N1N-C2N
2	A	2001	NDP	C5D-O5D-PN-O3
2	B	2002	NDP	C5B-O5B-PA-O3
2	C	2003	NDP	C3D-C4D-C5D-O5D
2	A	2001	NDP	C2B-O2B-P2B-O3X
2	C	2003	NDP	O4D-C1D-N1N-C2N
2	D	2004	NDP	O4D-C1D-N1N-C2N
2	D	2004	NDP	C4B-C5B-O5B-PA
2	A	2001	NDP	O4D-C1D-N1N-C2N
2	C	2003	NDP	C2N-C3N-C7N-N7N
2	C	2003	NDP	C2B-O2B-P2B-O1X
2	A	2001	NDP	C2D-C1D-N1N-C2N
2	D	2004	NDP	C2D-C1D-N1N-C2N
2	B	2002	NDP	O4D-C4D-C5D-O5D
2	A	2001	NDP	PN-O3-PA-O2A
2	C	2003	NDP	PN-O3-PA-O2A
2	D	2004	NDP	PN-O3-PA-O2A
2	B	2002	NDP	C3D-C4D-C5D-O5D
2	D	2004	NDP	C2B-O2B-P2B-O3X
2	C	2003	NDP	C2D-C1D-N1N-C2N
2	B	2002	NDP	C2B-O2B-P2B-O1X
2	D	2004	NDP	C2B-O2B-P2B-O1X
2	B	2002	NDP	PA-O3-PN-O2N

There are no ring outliers.

6 monomers are involved in 26 short contacts:

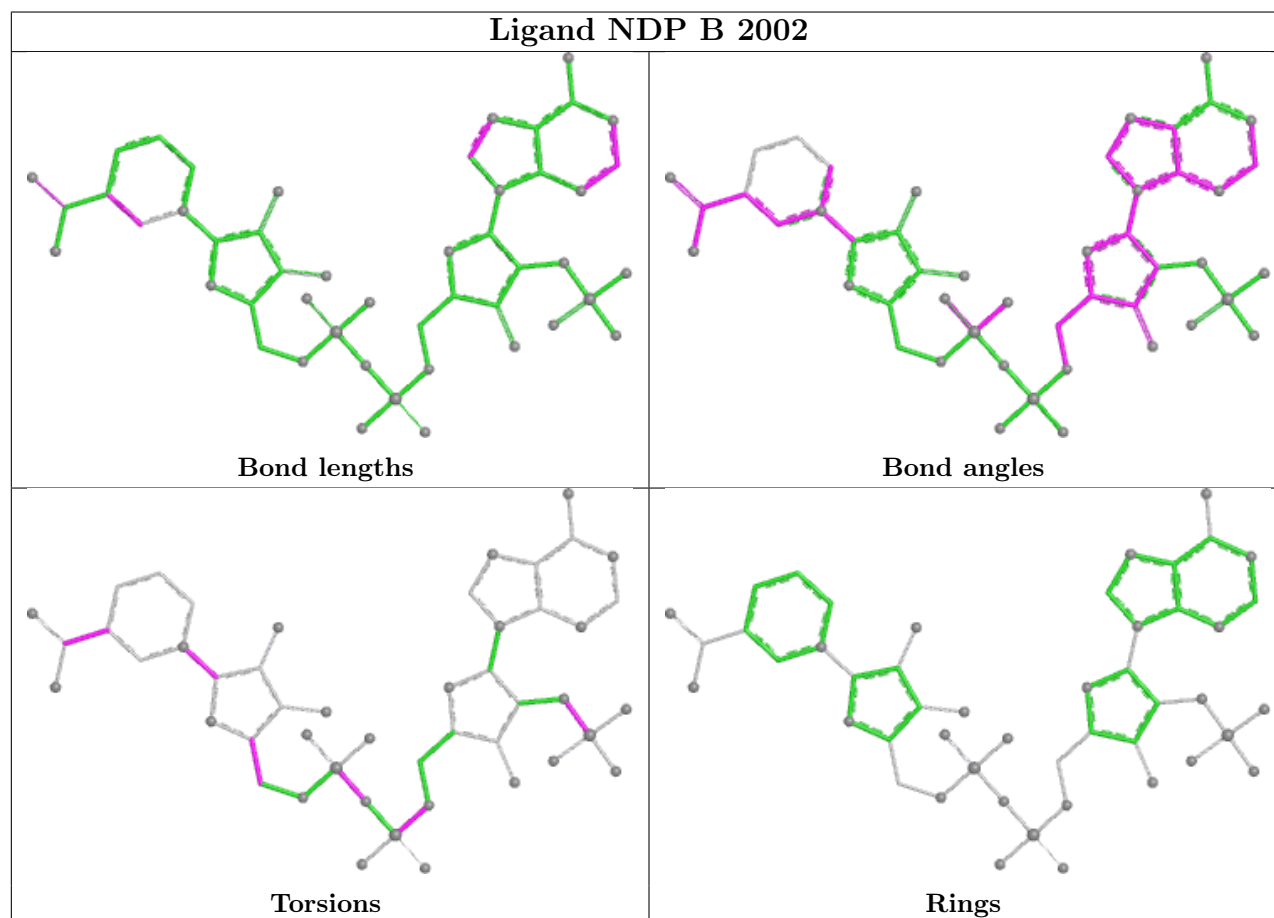
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	NDP	2	0

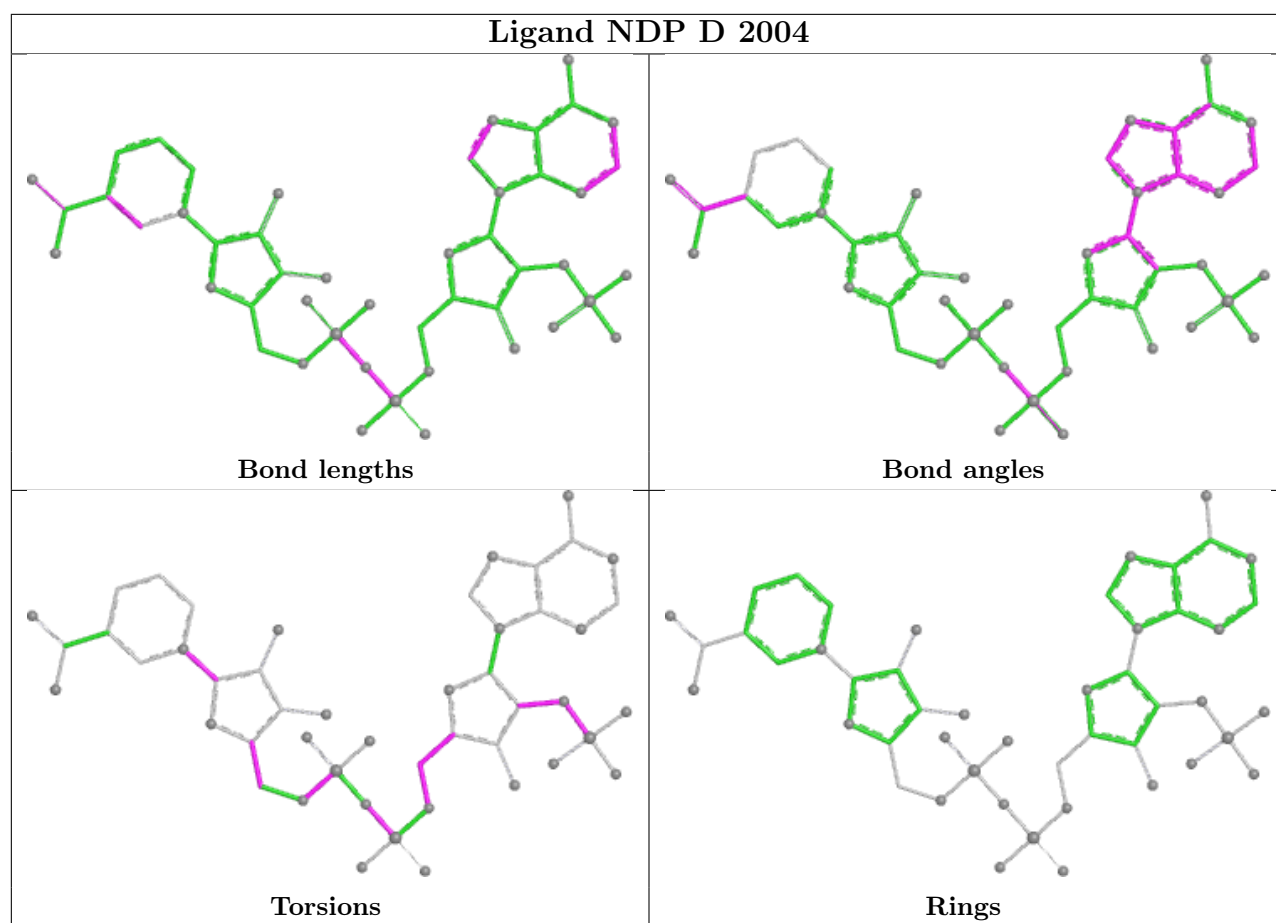
Continued on next page...

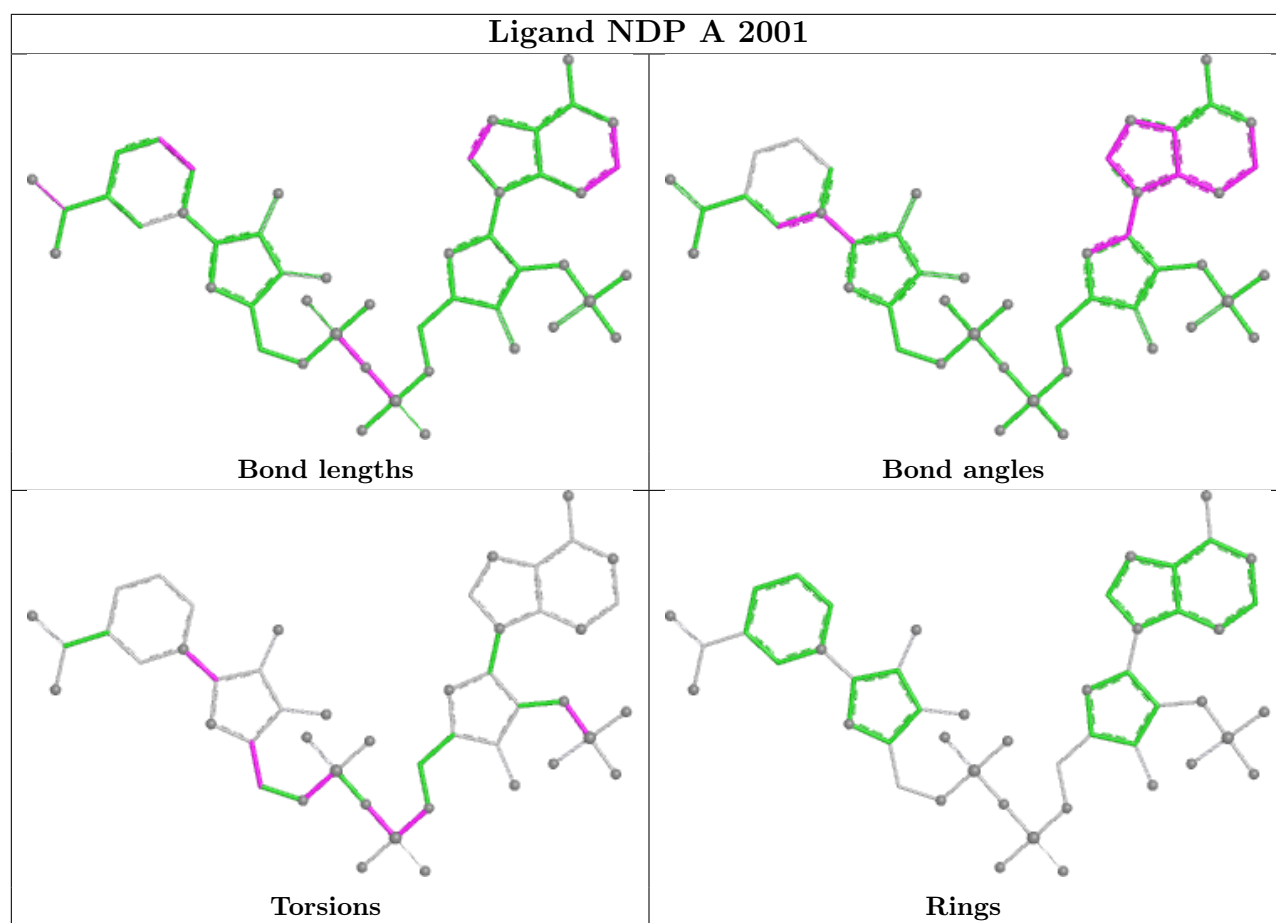
Continued from previous page...

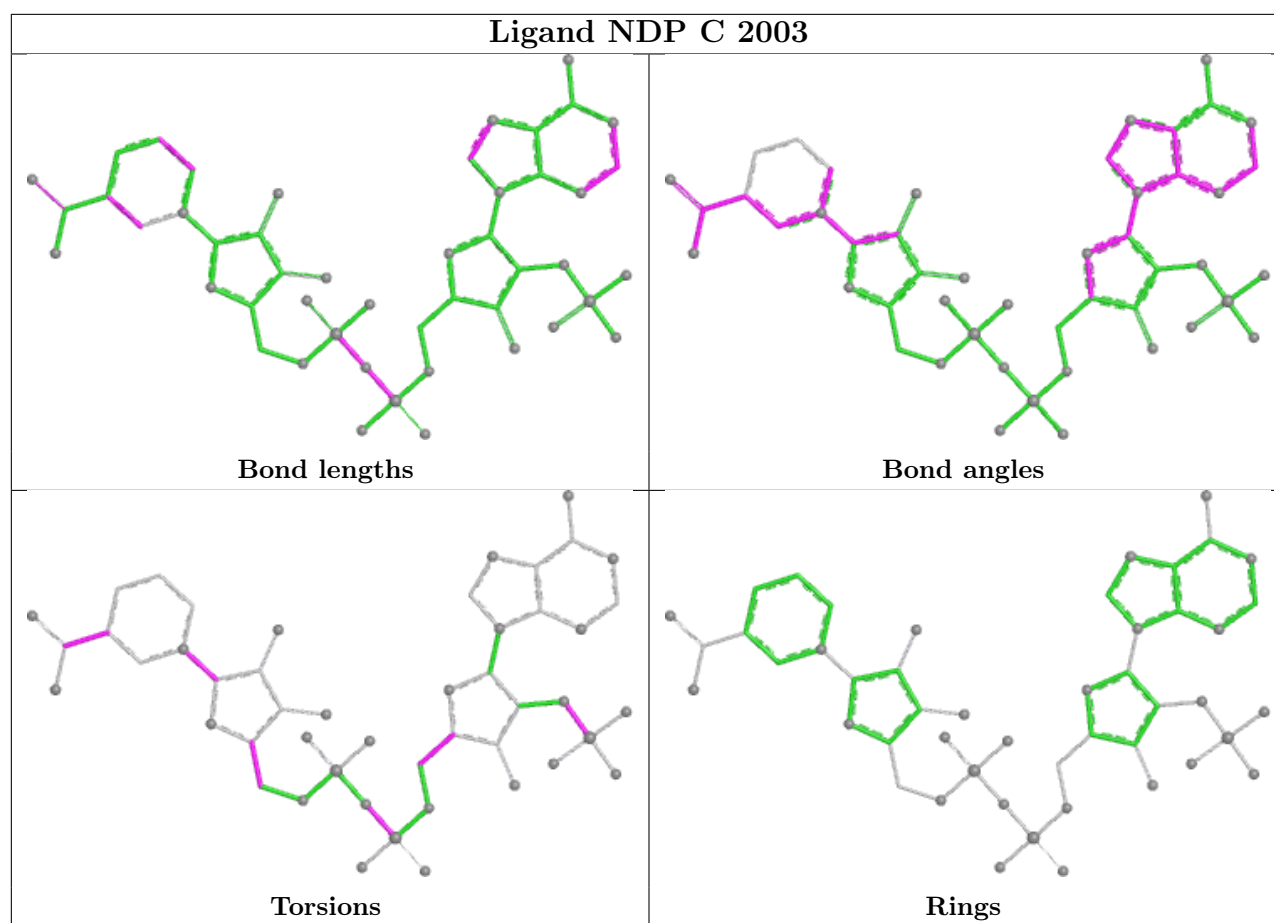
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2004	NDP	7	0
2	A	2001	NDP	10	0
3	A	3001	DGY	7	0
2	C	2003	NDP	4	0
3	C	3002	DGY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/330 (98%)	0.63	19 (5%) 28 25	19, 30, 39, 56	9 (2%)
1	B	323/330 (97%)	0.43	4 (1%) 76 74	16, 27, 36, 49	12 (3%)
1	C	324/330 (98%)	0.90	40 (12%) 8 6	16, 32, 43, 50	21 (6%)
1	D	323/330 (97%)	1.65	85 (26%) 1 1	5, 33, 50, 65	42 (13%)
All	All	1294/1320 (98%)	0.90	148 (11%) 10 7	5, 31, 43, 65	84 (6%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	ALA	26.0
1	D	51	GLY	10.2
1	D	314	LEU	7.1
1	D	66	ARG	7.0
1	D	65	LYS	6.5
1	D	315	ALA	6.5
1	D	67	ILE	6.4
1	D	313	LEU	6.4
1	D	34	TRP	6.3
1	D	327	LYS	6.3
1	D	318	ARG	6.2
1	D	89	ALA	6.0
1	D	73	ALA	5.9
1	D	88	LEU	5.7
1	D	70	ALA	5.7
1	D	63	VAL	5.7
1	D	319	GLY	5.1
1	D	75	LEU	4.7
1	D	42	ALA	4.7
1	D	64	ASP	4.6
1	D	90	LEU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	43	LYS	4.5
1	C	5	ARG	4.5
1	D	321	PRO	4.5
1	D	72	GLY	4.4
1	D	317	LEU	4.3
1	D	93	ILE	4.3
1	D	59	LEU	4.3
1	D	316	GLY	4.2
1	D	78	ILE	4.1
1	D	50	ALA	4.1
1	D	322	MET	4.1
1	D	91	ASP	4.0
1	C	174	PRO	4.0
1	C	169	ALA	3.8
1	D	26	ALA	3.8
1	C	185	ARG	3.8
1	D	49	VAL	3.7
1	C	188	ARG	3.7
1	C	199	PHE	3.6
1	D	53	HIS	3.6
1	D	74	ASN	3.6
1	D	6	LEU	3.5
1	C	161	LEU	3.5
1	D	69	ASP	3.5
1	D	45	LEU	3.5
1	A	5	ARG	3.5
1	D	60	SER	3.4
1	C	31	VAL	3.4
1	C	316	GLY	3.4
1	C	317	LEU	3.3
1	A	328	LEU	3.3
1	B	6	LEU	3.2
1	C	172	LEU	3.2
1	C	318	ARG	3.2
1	D	32	GLU	3.1
1	D	36	SER	3.1
1	D	86	ASP	3.1
1	D	326	LEU	3.1
1	C	159	ILE	3.1
1	D	31	VAL	3.1
1	C	168	ILE	3.1
1	D	62	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	21	VAL	3.0
1	D	20	ARG	3.0
1	D	44	GLU	3.0
1	C	177	VAL	2.9
1	C	154	SER	2.9
1	D	8	LYS	2.9
1	A	214	VAL	2.9
1	D	25	ARG	2.8
1	C	167	ALA	2.8
1	D	328	LEU	2.8
1	D	320	GLU	2.8
1	D	17	ALA	2.8
1	D	61	ASP	2.7
1	C	160	GLY	2.7
1	D	46	GLU	2.7
1	D	47	ARG	2.7
1	C	180	PHE	2.6
1	A	185	ARG	2.6
1	C	155	THR	2.6
1	D	103	THR	2.6
1	C	162	GLY	2.6
1	A	262	LYS	2.6
1	D	56	LEU	2.6
1	C	198	GLU	2.5
1	D	35	ASP	2.5
1	C	43	LYS	2.5
1	C	156	VAL	2.5
1	D	85	ILE	2.5
1	D	58	LEU	2.5
1	D	9	VAL	2.4
1	D	48	GLY	2.4
1	D	29	CYS	2.4
1	A	211	PHE	2.4
1	C	158	ILE	2.4
1	A	35	ASP	2.4
1	A	321	PRO	2.4
1	B	220	PRO	2.4
1	C	189	PRO	2.4
1	B	219	THR	2.4
1	A	324	SER	2.4
1	D	76	LYS	2.4
1	A	220	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	176	GLY	2.4
1	D	98	ILE	2.4
1	C	222	THR	2.3
1	D	100	VAL	2.3
1	D	55	LEU	2.3
1	A	167	ALA	2.3
1	D	95	LYS	2.3
1	D	19	GLY	2.3
1	D	325	GLU	2.3
1	D	243	ILE	2.3
1	C	171	ARG	2.3
1	A	243	ILE	2.3
1	D	83	VAL	2.3
1	A	152	THR	2.2
1	C	297	ALA	2.2
1	D	81	MET	2.2
1	C	320	GLU	2.2
1	A	264	ALA	2.2
1	D	309	ALA	2.2
1	A	149	TYR	2.2
1	C	144	LEU	2.2
1	A	213	VAL	2.2
1	D	41	PRO	2.2
1	C	197	ALA	2.2
1	D	22	ALA	2.2
1	D	54	GLY	2.1
1	D	97	GLY	2.1
1	C	192	ALA	2.1
1	C	221	ALA	2.1
1	D	96	ARG	2.1
1	D	99	ARG	2.1
1	C	326	LEU	2.1
1	A	189	PRO	2.1
1	C	145	TRP	2.1
1	C	232	GLN	2.1
1	A	215	ALA	2.1
1	C	140	SER	2.1
1	D	220	PRO	2.1
1	D	27	ALA	2.0
1	D	52	ALA	2.0
1	A	56	LEU	2.0
1	C	215	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

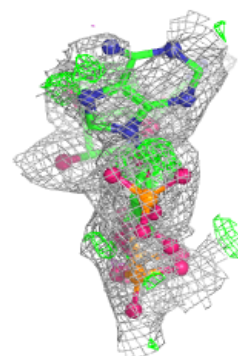
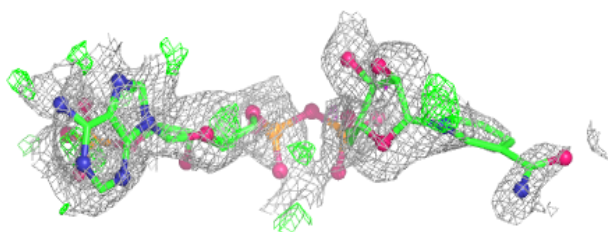
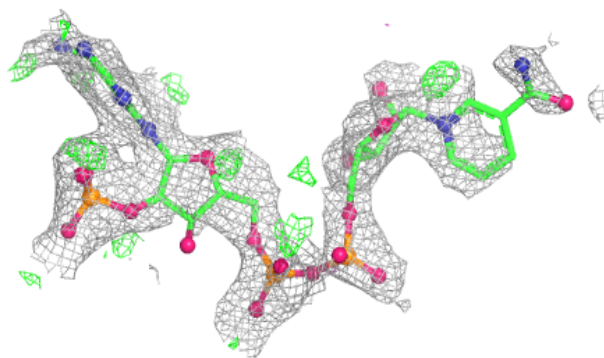
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	1001	5/5	0.64	0.20	110,110,110,111	0
2	NDP	D	2004	48/48	0.77	0.23	30,48,50,52	48
4	SO4	D	1002	5/5	0.77	0.17	86,87,88,88	0
4	SO4	D	1003	5/5	0.80	0.17	72,72,73,74	0
2	NDP	B	2002	48/48	0.82	0.19	17,30,40,42	48
2	NDP	C	2003	48/48	0.85	0.18	28,54,63,64	48
4	SO4	B	1005	5/5	0.86	0.15	78,79,80,80	0
4	SO4	D	1004	5/5	0.86	0.17	85,85,85,86	0
2	NDP	A	2001	48/48	0.87	0.16	31,53,58,59	48
3	DGY	C	3002	7/7	0.92	0.12	44,47,48,49	0
3	DGY	A	3001	7/7	0.92	0.19	38,40,43,44	0

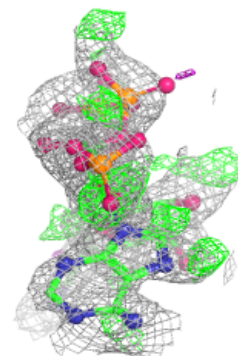
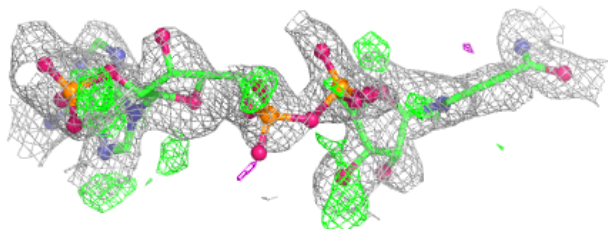
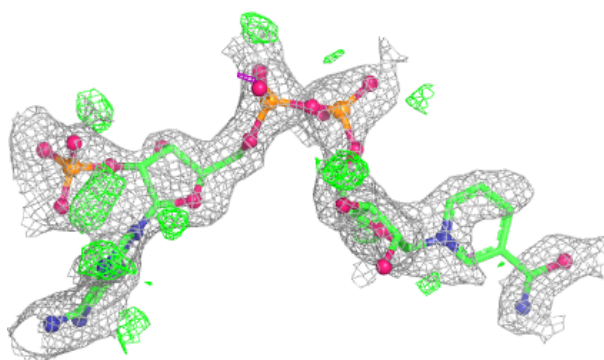
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NDP D 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

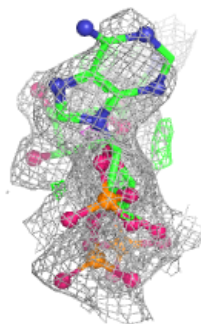
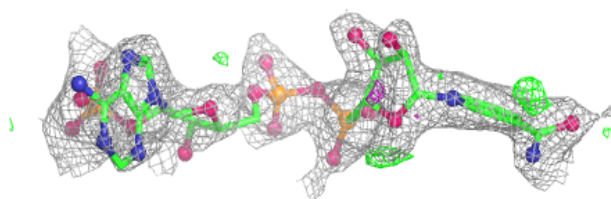
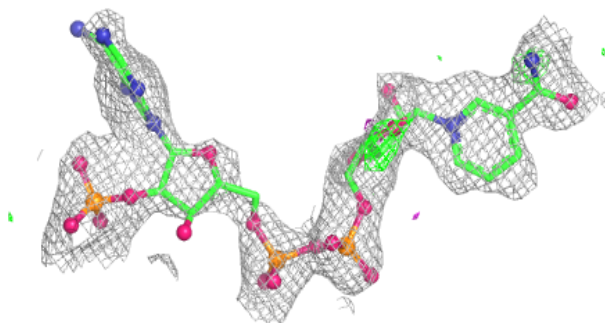
**Electron density around NDP B 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

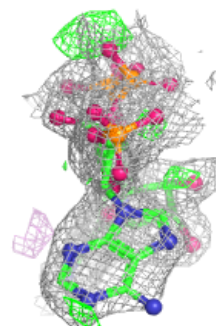
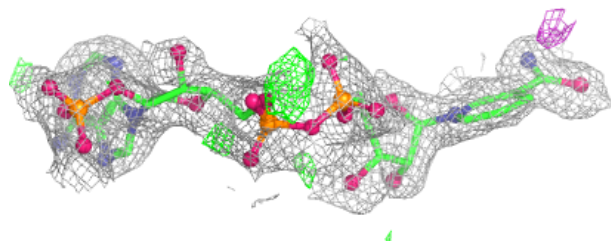
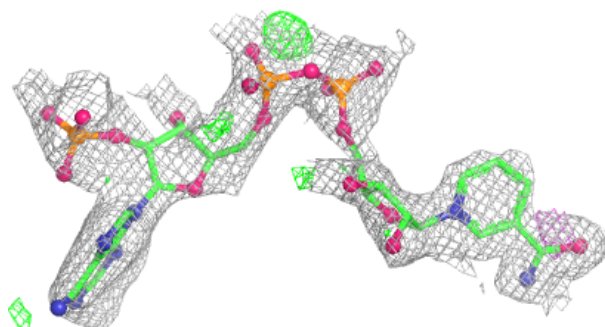


Electron density around NDP C 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NDP A 2001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.