Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NP9
Title	:	Crystal structure of a dioxygenase in the Crotonase superfamily
Authors	:	Bruner, S.D.; Widboom, P.F.; Fielding, E.N.
Deposited on	:	2006-10-26
Resolution	:	2.45 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.4%
Sidechain outliers		2.6%
RSRZ outliers		2.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
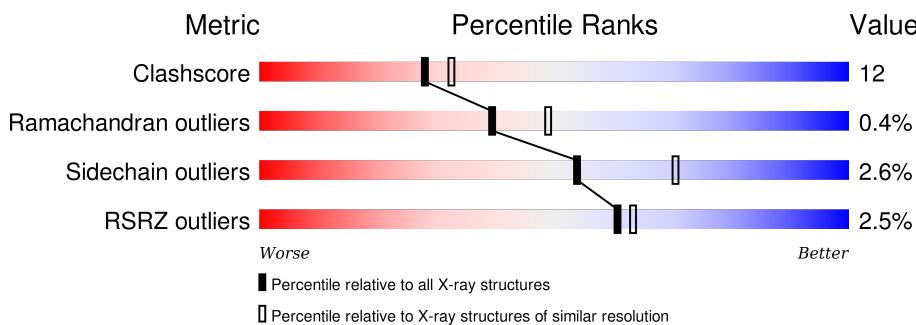
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	440	4% ▮ 74%	21% ··
1	B	440	% ▮ 73%	22% ··
1	C	440	2% ▮ 73%	22% ··
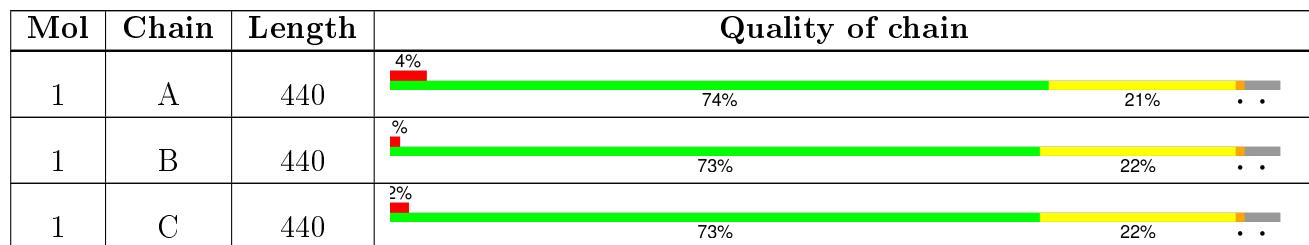
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXY	C	888	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10186 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 DpgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total 3250	C 2043	N 603	O 594	S 10	0	0	0
1	B	422	Total 3271	C 2054	N 610	O 597	S 10	0	0	0
1	C	421	Total 3258	C 2047	N 606	O 595	S 10	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	CLONING ARTIFACT	UNP Q8KLK7
A	0	MET	-	CLONING ARTIFACT	UNP Q8KLK7
A	1	GLY	-	CLONING ARTIFACT	UNP Q8KLK7
B	-1	ALA	-	CLONING ARTIFACT	UNP Q8KLK7
B	0	MET	-	CLONING ARTIFACT	UNP Q8KLK7
B	1	GLY	-	CLONING ARTIFACT	UNP Q8KLK7
C	-1	ALA	-	CLONING ARTIFACT	UNP Q8KLK7
C	0	MET	-	CLONING ARTIFACT	UNP Q8KLK7
C	1	GLY	-	CLONING ARTIFACT	UNP Q8KLK7

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHO NOOXY)TETRAHYDROFURAN-2-YL]METHYL (3R)-4-({3-[(2-{[(3,5-DIHYDROXYPH ENYL)ACETYL]AMINO}ETHYL)AMINO]-3-OXOPROPYL}AMINO)-3-HYDROXY-2, 2-DIMETHYL-4-OXOBUTYL DIHYDROGEN DIPHOSPHATE (three-letter code: YE1) (formula: $C_{29}H_{43}N_8O_{19}P_3$).
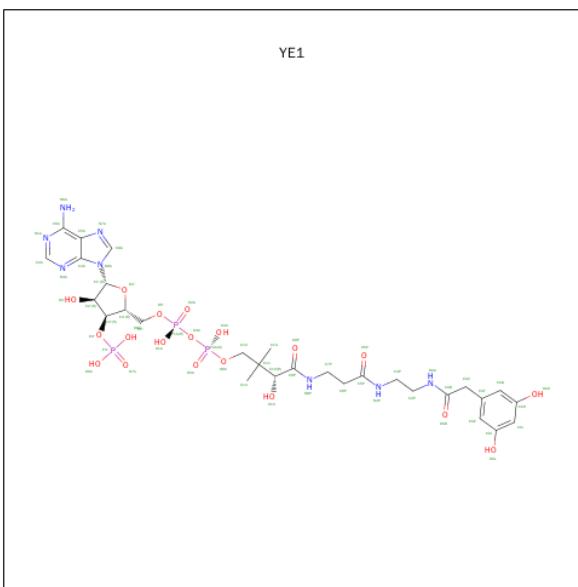
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
2	B	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
2	C	1	Total	C	N	O	P	0	0
			59	29	8	19	3		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).
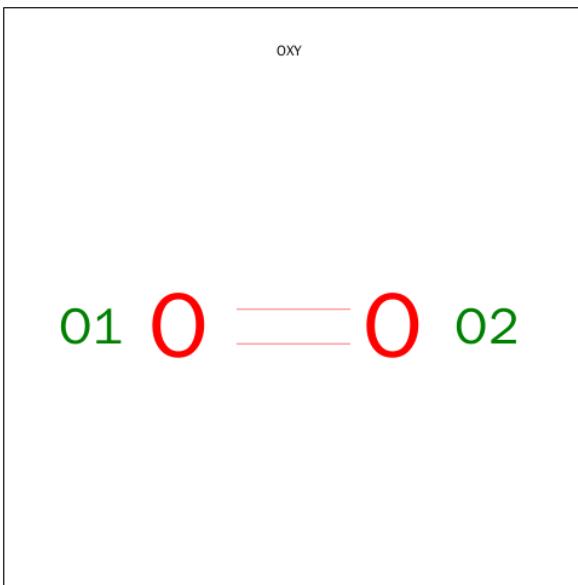
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 2	O 2	0	0
3	C	1	Total 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total 83	O 83	0	0
4	B	74	Total 74	O 74	0	0
4	C	67	Total 67	O 67	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DpgC
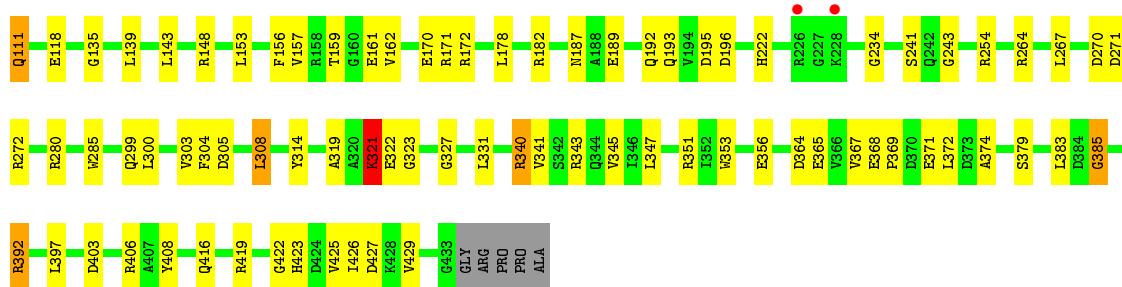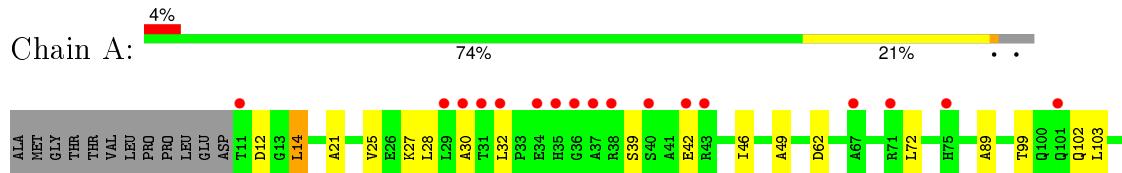
- Molecule 1: DpgC
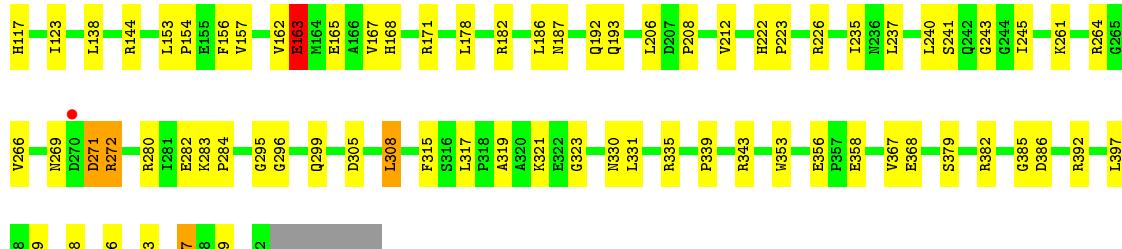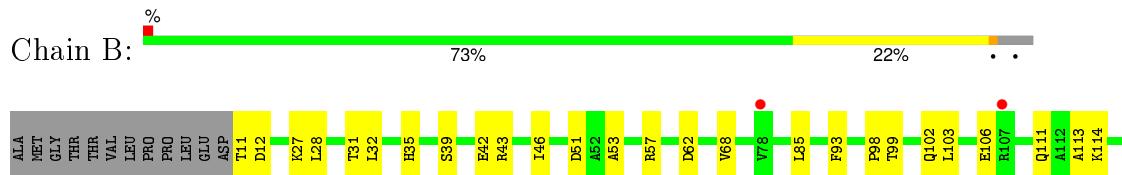
- Molecule 1: DpgC
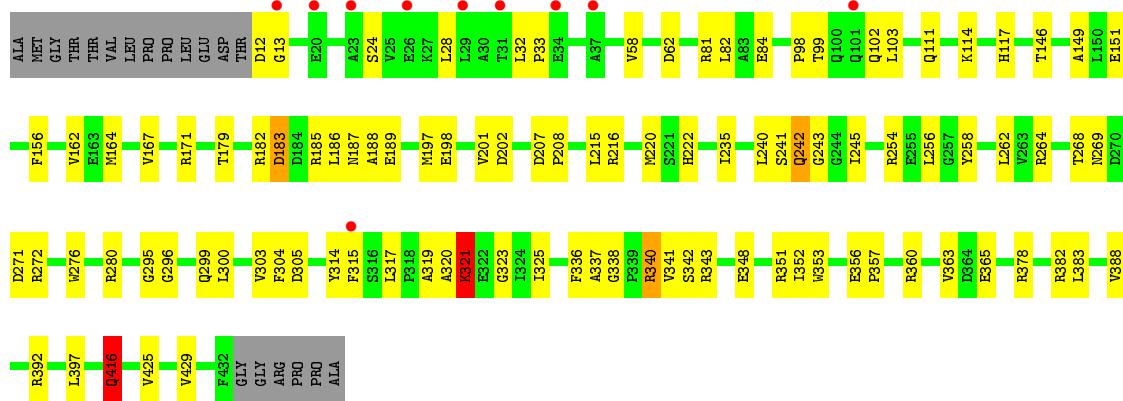
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.86Å 156.66Å 171.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 49.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.0 (50.00-2.45) 92.3 (49.90-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.49 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.328 , 0.356 0.343 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|>=0.50$, $<L^2>=0.34$	Xtriage
Outliers	4 of 143883 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	10186	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 22.95 % 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 5.1377e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: YE1, OXY

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	0.64	9/3310 (0.3%)	0.67	2/4490 (0.0%)
1	B	0.69	13/3332 (0.4%)	0.68	3/4517 (0.1%)
1	C	1.03	30/3319 (0.9%)	0.79	11/4500 (0.2%)
All	All	0.80	52/9961 (0.5%)	0.72	16/13507 (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	C	1	0

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	365	GLU	CD-OE1	-19.61	1.04	1.25
1	C	365	GLU	CD-OE2	-19.10	1.04	1.25
1	A	303	VAL	CB-CG2	-18.82	1.13	1.52
1	A	303	VAL	C-O	-13.97	0.96	1.23
1	B	163	GLU	C-O	-13.40	0.97	1.23
1	C	300	LEU	CG-CD2	-12.54	1.05	1.51
1	C	365	GLU	C-O	-12.52	0.99	1.23
1	C	416	GLN	C-O	-12.46	0.99	1.23
1	B	163	GLU	CB-CG	-12.43	1.28	1.52
1	C	416	GLN	CD-NE2	-12.06	1.02	1.32
1	B	321	LYS	C-O	-11.62	1.01	1.23
1	C	103	LEU	C-O	-11.21	1.02	1.23
1	C	300	LEU	C-O	-11.16	1.02	1.23
1	C	416	GLN	CD-OE1	-10.57	1.00	1.24
1	C	103	LEU	CG-CD1	-9.41	1.17	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	321	LYS	CA-C	-9.26	1.28	1.52
1	C	321	LYS	N-CA	-8.83	1.28	1.46
1	A	303	VAL	CB-CG1	-8.70	1.34	1.52
1	B	163	GLU	CA-CB	-8.70	1.34	1.53
1	B	103	LEU	CA-C	-8.32	1.31	1.52
1	B	163	GLU	CG-CD	-7.99	1.40	1.51
1	C	321	LYS	CB-CG	-7.90	1.31	1.52
1	C	151	GLU	C-O	-7.62	1.08	1.23
1	C	242	GLN	C-O	-7.51	1.09	1.23
1	C	300	LEU	CG-CD1	-7.37	1.24	1.51
1	C	365	GLU	CA-CB	-7.28	1.38	1.53
1	C	242	GLN	CD-OE1	-7.20	1.08	1.24
1	B	103	LEU	CG-CD2	-7.19	1.25	1.51
1	C	321	LYS	C-O	-7.09	1.09	1.23
1	C	151	GLU	N-CA	-7.01	1.32	1.46
1	C	151	GLU	CA-CB	-6.83	1.39	1.53
1	B	321	LYS	N-CA	-6.78	1.32	1.46
1	B	321	LYS	CA-CB	-6.73	1.39	1.53
1	B	163	GLU	N-CA	-6.63	1.33	1.46
1	C	300	LEU	N-CA	-6.52	1.33	1.46
1	A	321	LYS	C-O	-6.44	1.11	1.23
1	C	416	GLN	CG-CD	-6.34	1.36	1.51
1	C	321	LYS	CA-CB	-6.24	1.40	1.53
1	C	242	GLN	CD-NE2	-6.19	1.17	1.32
1	C	103	LEU	CG-CD2	-6.18	1.28	1.51
1	C	365	GLU	N-CA	-5.97	1.34	1.46
1	A	103	LEU	CG-CD1	-5.97	1.29	1.51
1	C	416	GLN	N-CA	-5.69	1.34	1.46
1	B	163	GLU	CA-C	-5.64	1.38	1.52
1	C	300	LEU	C-N	-5.55	1.21	1.34
1	B	103	LEU	C-O	-5.53	1.12	1.23
1	B	163	GLU	CD-OE1	-5.40	1.19	1.25
1	A	103	LEU	C-O	-5.22	1.13	1.23
1	A	103	LEU	CG-CD2	-5.19	1.32	1.51
1	A	303	VAL	CA-C	-5.16	1.39	1.52
1	A	321	LYS	CD-CE	-5.15	1.38	1.51
1	C	320	ALA	C-N	-5.10	1.22	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	LEU	CA-CB-CG	15.10	150.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	CA-CB-CG	11.00	140.60	115.30
1	C	365	GLU	OE1-CD-OE2	-10.19	111.07	123.30
1	C	321	LYS	N-CA-C	9.18	135.80	111.00
1	C	103	LEU	CA-CB-CG	8.29	134.37	115.30
1	A	303	VAL	CA-CB-CG1	6.96	121.34	110.90
1	C	151	GLU	CA-CB-CG	6.93	128.64	113.40
1	C	151	GLU	N-CA-CB	-6.79	98.38	110.60
1	C	317	LEU	N-CA-C	-6.12	94.47	111.00
1	B	103	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	317	LEU	N-CA-C	-5.88	95.11	111.00
1	C	103	LEU	CB-CG-CD2	5.71	120.72	111.00
1	C	365	GLU	CG-CD-OE1	5.28	128.87	118.30
1	C	151	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	C	365	GLU	CA-CB-CG	5.15	124.73	113.40
1	B	321	LYS	N-CA-C	5.04	124.61	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	321	LYS	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3250	0	3248	74	0
1	B	3271	0	3280	68	0
1	C	3258	0	3261	77	0
2	A	59	0	37	10	0
2	B	59	0	37	8	0
2	C	59	0	37	9	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	83	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	74	0	0	4	0
4	C	67	0	0	3	0
All	All	10186	0	9900	233	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 12.

All (233) 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:A:241:SER:HB2	1:A:429:VAL:HG12	1.47	0.94
1:A:159:THR:HG22	1:A:161:GLU:H	1.31	0.93
1:C:241:SER:HB2	1:C:429:VAL:HG12	1.52	0.91
1:C:319:ALA:HB1	1:C:323:GLY:HA3	1.55	0.88
1:A:159:THR:HG21	4:A:1055:HOH:O	1.73	0.87
1:B:319:ALA:HB1	1:B:323:GLY:HA3	1.55	0.86
1:B:241:SER:HB2	1:B:429:VAL:HG12	1.58	0.84
1:B:99:THR:OG1	1:B:102:GLN:HG3	1.80	0.81
1:A:12:ASP:OD2	1:A:14:LEU:HB2	1.83	0.79
1:B:165:GLU:OE1	1:B:192:GLN:HG2	1.83	0.78
1:C:99:THR:OG1	1:C:102:GLN:HG3	1.82	0.78
1:A:99:THR:OG1	1:A:102:GLN:HB2	1.84	0.77
1:C:99:THR:H	1:C:102:GLN:HE21	1.33	0.77
1:A:159:THR:HG22	1:A:161:GLU:N	2.00	0.76
1:A:419:ARG:O	1:A:425:VAL:HG11	1.85	0.76
1:C:99:THR:H	1:C:102:GLN:NE2	1.84	0.75
1:C:182:ARG:HG3	4:C:1035:HOH:O	1.87	0.74
1:B:271:ASP:OD1	1:B:272:ARG:HG2	1.87	0.74
1:A:182:ARG:HB2	1:A:187:ASN:HA	1.68	0.74
1:C:378:ARG:HG2	1:C:382:ARG:NH1	2.02	0.74
1:C:146:THR:HG23	1:C:149:ALA:H	1.53	0.73
1:C:325:ILE:H	1:C:416:GLN:HE22	1.37	0.72
2:A:999:YE1:O9A	2:A:999:YE1:O2'	2.04	0.72
2:B:999:YE1:O2'	2:B:999:YE1:O9A	2.08	0.69
1:A:182:ARG:HG3	4:A:1011:HOH:O	1.93	0.69
1:C:99:THR:HG23	1:C:102:GLN:HE21	1.58	0.68
1:B:212:VAL:HG22	1:B:284:PRO:HG2	1.76	0.68
1:B:305:ASP:OD1	1:B:392:ARG:HD2	1.93	0.67
1:C:82:LEU:HD11	1:C:256:LEU:HD12	1.75	0.67
2:C:999:YE1:HAE	2:C:999:YE1:OAD	1.95	0.67
1:B:385:GLY:HA3	4:B:1043:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:CG	1:B:163:GLU:O	2.29	0.66
2:A:999:YE1:HAE	2:A:999:YE1:OAD	1.95	0.66
2:B:999:YE1:OAD	2:B:999:YE1:HAE	1.95	0.65
1:A:25:VAL:HG22	1:A:49:ALA:HB1	1.78	0.65
1:C:319:ALA:CB	1:C:323:GLY:HA3	2.27	0.65
1:B:182:ARG:HB2	1:B:187:ASN:HA	1.78	0.64
1:C:111:GLN:HG2	1:C:243:GLY:HA2	1.80	0.63
1:A:422:GLY:O	1:A:426:ILE:HG13	1.98	0.63
1:C:378:ARG:HG2	1:C:382:ARG:HH12	1.61	0.63
1:B:111:GLN:HE21	1:B:243:GLY:HA2	1.63	0.63
1:A:170:GLU:OE2	1:A:172:ARG:HD3	1.99	0.63
2:A:999:YE1:O10	2:A:999:YE1:HC8	2.01	0.61
1:A:425:VAL:O	1:A:429:VAL:HG23	2.00	0.61
1:A:118:GLU:HG3	4:A:1078:HOH:O	2.00	0.61
1:B:99:THR:H	1:B:102:GLN:HE21	1.49	0.60
2:C:999:YE1:O10	2:C:999:YE1:HC8	2.02	0.60
1:A:254:ARG:HD3	2:A:999:YE1:HAI	1.84	0.60
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.66	0.60
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.67	0.60
1:C:357:PRO:O	1:C:360:ARG:HG2	2.01	0.59
1:C:314:TYR:CD2	1:C:351:ARG:HD2	2.38	0.59
1:B:226:ARG:HH11	1:B:226:ARG:HG3	1.68	0.58
1:B:385:GLY:CA	4:B:1043:HOH:O	2.48	0.58
2:A:999:YE1:C8A	2:A:999:YE1:O10	2.51	0.58
2:A:999:YE1:C8A	2:A:999:YE1:HO10	2.17	0.58
1:C:264:ARG:HH11	1:C:264:ARG:HG2	1.68	0.58
1:A:308:LEU:CD1	1:A:365:GLU:HB2	2.33	0.58
1:A:39:SER:OG	1:A:42:GLU:HG3	2.02	0.58
1:A:397:LEU:HD23	1:A:397:LEU:C	2.24	0.58
1:A:308:LEU:N	1:A:308:LEU:HD22	2.19	0.57
1:C:12:ASP:CG	1:C:13:GLY:H	2.08	0.57
1:A:343:ARG:O	1:A:347:LEU:HB2	2.04	0.57
1:C:319:ALA:HB1	1:C:323:GLY:CA	2.33	0.57
2:B:999:YE1:C8A	2:B:999:YE1:HO10	2.18	0.57
1:C:295:GLY:O	1:C:299:GLN:HG3	2.04	0.57
1:C:99:THR:HG23	1:C:102:GLN:NE2	2.20	0.56
2:C:999:YE1:O10	2:C:999:YE1:C8A	2.53	0.56
2:C:999:YE1:HO10	2:C:999:YE1:C8A	2.17	0.56
1:A:308:LEU:HD13	1:A:365:GLU:HB2	1.87	0.56
1:C:353:TRP:O	1:C:356:GLU:HG2	2.05	0.56
1:B:222:HIS:CD2	2:B:999:YE1:H4'	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:SER:HB2	4:A:1043:HOH:O	2.06	0.56
1:A:153:LEU:O	1:A:157:VAL:HG23	2.06	0.55
1:A:135:GLY:HA3	1:A:406:ARG:HD2	1.87	0.54
1:C:268:THR:OG1	1:C:272:ARG:NH1	2.37	0.54
1:C:222:HIS:CD2	2:C:999:YE1:H4'	2.43	0.54
1:C:28:LEU:O	1:C:28:LEU:HD23	2.07	0.54
1:B:339:PRO:HG2	1:C:336:PHE:CD1	2.43	0.54
1:C:111:GLN:HG3	1:C:240:LEU:O	2.08	0.54
1:A:340:ARG:HA	1:A:340:ARG:NH1	2.23	0.54
1:A:178:LEU:HD12	1:A:178:LEU:N	2.24	0.53
1:A:285:TRP:HB3	1:A:304:PHE:CE1	2.44	0.53
1:A:222:HIS:CD2	2:A:999:YE1:H4'	2.43	0.53
1:C:262:LEU:O	1:C:392:ARG:NH2	2.38	0.53
2:B:999:YE1:C8A	2:B:999:YE1:O10	2.57	0.53
2:B:999:YE1:HC8	2:B:999:YE1:O10	2.08	0.53
1:C:81:ARG:HB2	1:C:84:GLU:OE1	2.09	0.53
1:C:32:LEU:HG	1:C:33:PRO:HD2	1.91	0.52
1:B:106:GLU:O	1:B:114:LYS:HE2	2.08	0.52
1:A:321:LYS:C	1:A:322:GLU:HG3	2.29	0.52
1:A:234:GLY:HA3	2:A:999:YE1:HC22	1.92	0.52
1:B:416:GLN:HA	1:B:416:GLN:OE1	2.09	0.51
1:A:111:GLN:HG2	1:A:243:GLY:HA2	1.92	0.51
1:A:299:GLN:OE1	1:A:327:GLY:HA3	2.10	0.51
1:B:39:SER:O	1:B:43:ARG:HG3	2.11	0.51
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.26	0.51
1:C:146:THR:HG22	1:C:202:ASP:OD2	2.11	0.51
1:B:331:LEU:HB2	1:B:408:TYR:CD1	2.45	0.51
1:A:331:LEU:HB2	1:A:408:TYR:CD1	2.46	0.51
1:C:111:GLN:HE21	1:C:243:GLY:HA2	1.77	0.50
1:C:99:THR:HG1	1:C:102:GLN:HG3	1.76	0.50
1:B:28:LEU:O	1:B:32:LEU:HB2	2.10	0.50
1:C:264:ARG:NH1	4:C:1062:HOH:O	2.42	0.50
1:A:182:ARG:CG	4:A:1011:HOH:O	2.56	0.50
1:B:98:PRO:HG3	1:B:117:HIS:HB3	1.93	0.49
1:A:305:ASP:OD2	1:A:392:ARG:NH1	2.46	0.49
1:A:314:TYR:CD2	1:A:351:ARG:HD2	2.46	0.49
1:A:341:VAL:O	1:A:345:VAL:HG23	2.13	0.49
1:C:235:ILE:HB	2:C:999:YE1:HAE	1.94	0.49
1:A:157:VAL:O	1:A:171:ARG:NH2	2.46	0.49
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.77	0.49
1:B:226:ARG:HG3	1:B:226:ARG:NH1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LYS:HE2	1:C:321:LYS:HB3	1.61	0.48
1:C:189:GLU:OE1	2:C:999:YE1:OAL	2.32	0.48
1:B:235:ILE:HB	2:B:999:YE1:HAE	1.96	0.47
1:A:423:HIS:O	1:A:427:ASP:HB2	2.13	0.47
1:A:422:GLY:O	1:A:425:VAL:HG12	2.13	0.47
1:C:343:ARG:HH11	1:C:343:ARG:HG3	1.80	0.47
1:B:358:GLU:HG3	4:B:1041:HOH:O	2.15	0.47
1:B:367:VAL:HG12	1:B:368:GLU:O	2.14	0.47
1:A:319:ALA:HB1	1:A:323:GLY:HA3	1.96	0.47
1:C:182:ARG:HB2	1:C:187:ASN:HA	1.95	0.47
1:C:198:GLU:HA	1:C:258:TYR:HB3	1.96	0.47
1:B:153:LEU:O	1:B:157:VAL:HG23	2.14	0.47
1:B:11:THR:HG23	1:B:12:ASP:N	2.30	0.47
1:B:35:HIS:CD2	1:B:113:ALA:HA	2.49	0.47
1:C:215:LEU:HD23	1:C:304:PHE:CZ	2.50	0.47
1:A:371:GLU:OE2	1:A:374:ALA:HB3	2.15	0.47
1:C:315:PHE:N	1:C:315:PHE:CD1	2.83	0.47
1:A:385:GLY:HA3	4:C:1002:HOH:O	2.15	0.47
1:A:383:LEU:HD21	1:C:348:GLU:OE2	2.16	0.46
1:A:156:PHE:CD1	1:A:162:VAL:HG23	2.51	0.46
2:C:999:YE1:O9A	2:C:999:YE1:O2'	2.23	0.46
1:B:156:PHE:CD1	1:B:162:VAL:HG23	2.50	0.46
1:C:197:MET:O	1:C:201:VAL:HG23	2.15	0.46
1:C:315:PHE:CZ	1:C:363:VAL:HG21	2.50	0.46
1:C:269:ASN:HB2	1:C:271:ASP:OD2	2.15	0.46
1:C:416:GLN:HE21	1:C:416:GLN:HA	1.81	0.46
1:A:397:LEU:HD23	1:A:397:LEU:O	2.16	0.46
1:A:403:ASP:HB2	4:A:1047:HOH:O	2.16	0.46
1:A:416:GLN:HA	1:A:416:GLN:OE1	2.16	0.46
1:A:156:PHE:HD1	1:A:162:VAL:HG23	1.81	0.46
1:B:53:ALA:O	1:B:57:ARG:HG3	2.15	0.46
1:A:367:VAL:HG13	1:A:372:LEU:HD13	1.96	0.46
1:B:42:GLU:O	1:B:46:ILE:HG22	2.16	0.45
2:A:999:YE1:CAE	2:A:999:YE1:OAD	2.62	0.45
1:B:123:ILE:HD11	1:C:276:TRP:CZ3	2.52	0.45
1:C:305:ASP:OD2	1:C:392:ARG:NH1	2.49	0.45
1:A:148:ARG:NH1	1:A:195:ASP:OD1	2.49	0.45
1:A:343:ARG:HG3	1:A:343:ARG:HH11	1.82	0.45
1:B:330:ASN:HB2	1:B:408:TYR:OH	2.17	0.45
1:C:24:SER:O	1:C:28:LEU:HB2	2.17	0.45
1:B:68:VAL:HG13	1:B:93:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ALA:HB1	1:C:341:VAL:HB	1.99	0.45
1:A:28:LEU:HG	1:A:32:LEU:CD1	2.46	0.45
1:A:27:LYS:O	1:A:30:ALA:HB3	2.16	0.45
2:C:999:YE1:OAD	2:C:999:YE1:CAE	2.62	0.44
1:A:46:ILE:O	1:A:49:ALA:HB3	2.17	0.44
1:C:183:ASP:HA	1:C:220:MET:SD	2.58	0.44
1:C:425:VAL:O	1:C:429:VAL:HG23	2.17	0.44
1:B:163:GLU:HG2	1:B:163:GLU:O	2.15	0.44
1:B:153:LEU:N	1:B:154:PRO:HD2	2.32	0.44
1:C:171:ARG:HD3	1:C:207:ASP:OD2	2.18	0.44
2:B:999:YE1:CAE	2:B:999:YE1:OAD	2.62	0.44
1:C:338:GLY:O	1:C:342:SER:HB2	2.17	0.44
1:B:319:ALA:CB	1:B:323:GLY:HA3	2.39	0.44
1:B:237:LEU:O	1:B:429:VAL:CG1	2.66	0.44
1:B:162:VAL:HG12	1:B:163:GLU:N	2.33	0.44
1:B:85:LEU:HD22	1:B:138:LEU:HD13	1.99	0.44
1:A:192:GLN:NE2	1:A:196:ASP:OD1	2.51	0.44
1:C:240:LEU:HA	1:C:245:ILE:HG12	1.99	0.43
1:A:308:LEU:CD2	1:A:308:LEU:N	2.81	0.43
1:A:305:ASP:CG	1:A:392:ARG:HH11	2.22	0.43
1:C:296:GLY:HA2	1:C:299:GLN:CD	2.38	0.43
1:B:261:LYS:HE2	1:B:266:VAL:HG12	2.00	0.43
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.83	0.43
1:A:353:TRP:O	1:A:356:GLU:HG2	2.19	0.43
1:B:235:ILE:HD11	1:B:245:ILE:HG21	2.00	0.43
1:B:343:ARG:HH11	1:B:343:ARG:HG3	1.83	0.43
1:C:207:ASP:HA	1:C:208:PRO:HD3	1.93	0.43
1:A:321:LYS:O	1:A:322:GLU:HG3	2.19	0.43
1:B:423:HIS:O	1:B:427:ASP:HB2	2.18	0.43
1:B:296:GLY:HA2	1:B:299:GLN:NE2	2.34	0.43
1:A:189:GLU:OE1	2:A:999:YE1:OAL	2.37	0.43
1:C:111:GLN:NE2	1:C:114:LYS:NZ	2.67	0.43
1:C:305:ASP:CG	1:C:392:ARG:HH11	2.23	0.43
1:C:264:ARG:O	1:C:280:ARG:HD2	2.19	0.42
1:B:222:HIS:CG	1:B:223:PRO:HD2	2.53	0.42
1:A:12:ASP:OD2	1:A:14:LEU:HD22	2.19	0.42
1:B:178:LEU:N	1:B:178:LEU:HD12	2.35	0.42
1:B:167:VAL:HG12	1:B:168:HIS:N	2.35	0.42
1:B:27:LYS:O	1:B:31:THR:HG23	2.19	0.42
1:A:364:ASP:OD1	1:C:340:ARG:HD3	2.20	0.42
1:C:264:ARG:NH1	1:C:264:ARG:HG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:HA	1:B:382:ARG:NH1	2.35	0.42
1:B:266:VAL:O	1:B:280:ARG:HA	2.19	0.42
1:B:335:ARG:HD3	1:B:399:ASP:HB3	2.02	0.42
1:A:21:ALA:O	1:A:25:VAL:HG23	2.19	0.42
1:B:282:GLU:O	1:B:283:LYS:HG3	2.20	0.42
1:A:72:LEU:HD11	1:A:89:ALA:HB2	2.01	0.42
1:B:264:ARG:NH1	1:B:264:ARG:HG2	2.35	0.42
1:A:368:GLU:OE1	1:A:369:PRO:HD2	2.19	0.42
1:B:223:PRO:HA	1:B:226:ARG:HG2	2.00	0.41
1:B:379:SER:HA	1:B:382:ARG:CZ	2.50	0.41
1:A:264:ARG:NH1	1:A:264:ARG:HG2	2.33	0.41
1:C:28:LEU:O	1:C:32:LEU:HB2	2.21	0.41
1:B:295:GLY:HA2	4:B:1035:HOH:O	2.20	0.41
1:C:185:ARG:HG3	1:C:188:ALA:H	1.86	0.41
1:A:72:LEU:HD21	1:A:89:ALA:HA	2.01	0.41
1:A:139:LEU:O	1:A:143:LEU:HG	2.21	0.41
1:B:353:TRP:O	1:B:356:GLU:HG2	2.20	0.41
1:B:11:THR:HG23	1:B:12:ASP:H	1.84	0.41
1:C:183:ASP:HA	1:C:220:MET:CE	2.51	0.41
1:C:383:LEU:HA	1:C:388:VAL:HG21	2.03	0.41
1:C:98:PRO:CG	1:C:117:HIS:HB3	2.50	0.41
1:B:206:LEU:O	1:B:208:PRO:HD3	2.21	0.41
1:C:179:THR:HA	1:C:216:ARG:O	2.21	0.41
1:C:58:VAL:HG12	1:C:62:ASP:OD2	2.20	0.41
1:C:156:PHE:CD1	1:C:162:VAL:HG23	2.55	0.41
1:B:144:ARG:NH2	1:B:269:ASN:OD1	2.54	0.41
1:C:164:MET:HB2	1:C:167:VAL:O	2.21	0.41
1:B:240:LEU:O	1:B:240:LEU:HD23	2.21	0.40
1:C:254:ARG:HH12	1:C:299:GLN:NE2	2.19	0.40
1:B:282:GLU:C	1:B:283:LYS:HG3	2.41	0.40
1:A:72:LEU:CD1	1:A:89:ALA:HB2	2.51	0.40
1:C:397:LEU:O	1:C:397:LEU:HD23	2.22	0.40
1:C:111:GLN:NE2	1:C:114:LYS:CE	2.85	0.40
1:B:111:GLN:HG3	1:B:240:LEU:O	2.21	0.40
1:B:308:LEU:CD2	1:B:308:LEU:N	2.85	0.40
1:B:157:VAL:HA	1:B:171:ARG:NH2	2.36	0.40
1:C:315:PHE:HD1	1:C:352:ILE:O	2.05	0.40
1:A:267:LEU:HA	1:A:280:ARG:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/440 (96%)	401 (95%)	17 (4%)	3 (1%)	26	32
1	B	420/440 (96%)	393 (94%)	27 (6%)	0	100	100
1	C	419/440 (95%)	405 (97%)	12 (3%)	2 (0%)	34	41
All	All	1260/1320 (96%)	1199 (95%)	56 (4%)	5 (0%)	39	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	ASP
1	A	111	GLN
1	A	270	ASP
1	C	242	GLN
1	A	385	GLY

5.3.2 Protein sidechains (i)

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	325/345 (94%)	316 (97%)	9 (3%)	51	68
1	B	330/345 (96%)	318 (96%)	12 (4%)	42	58
1	C	328/345 (95%)	323 (98%)	5 (2%)	72	84
All	All	983/1035 (95%)	957 (97%)	26 (3%)	54	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	62	ASP
1	A	193	GLN
1	A	271	ASP
1	A	300	LEU
1	A	308	LEU
1	A	321	LYS
1	A	340	ARG
1	A	392	ARG
1	B	51	ASP
1	B	62	ASP
1	B	163	GLU
1	B	186	LEU
1	B	193	GLN
1	B	271	ASP
1	B	272	ARG
1	B	308	LEU
1	B	315	PHE
1	B	386	ASP
1	B	397	LEU
1	B	427	ASP
1	C	186	LEU
1	C	303	VAL
1	C	321	LYS
1	C	340	ARG
1	C	416	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	102	GLN
1	A	111	GLN
1	A	193	GLN
1	B	35	HIS
1	B	64	HIS
1	B	102	GLN
1	B	111	GLN
1	B	117	HIS
1	B	193	GLN
1	B	423	HIS
1	C	102	GLN
1	C	111	GLN

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Mol	Chain	Res	Type
1	C	299	GLN
1	C	416	GLN

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 ⓘ

6 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	OXY	A	888	-	1,1,1	0.29	0	0,0,0	0.00	-
2	YE1	A	999	-	52,62,62	1.82	8 (15%)	68,92,92	2.34	17 (25%)
3	OXY	B	888	-	1,1,1	0.29	0	0,0,0	0.00	-
2	YE1	B	999	-	52,62,62	1.83	8 (15%)	68,92,92	2.34	17 (25%)
3	OXY	C	888	-	1,1,1	0.29	0	0,0,0	0.00	-
2	YE1	C	999	-	52,62,62	1.83	8 (15%)	68,92,92	2.34	17 (25%)

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	OXY	A	888	-	-	0/0/0/0	0/0/0/0
2	YE1	A	999	-	-	0/51/71/71	0/4/4/4
3	OXY	B	888	-	-	0/0/0/0	0/0/0/0
2	YE1	B	999	-	-	0/51/71/71	0/4/4/4
3	OXY	C	888	-	-	0/0/0/0	0/0/0/0
2	YE1	C	999	-	-	0/51/71/71	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	YE1	C2P-NAA	-4.65	1.35	1.46
2	B	999	YE1	C2P-NAA	-4.64	1.35	1.46
2	A	999	YE1	C2P-NAA	-4.63	1.35	1.46
2	B	999	YE1	C3P-N4P	-2.42	1.40	1.46
2	A	999	YE1	C3P-N4P	-2.42	1.40	1.46
2	C	999	YE1	C3P-N4P	-2.39	1.40	1.46
2	B	999	YE1	P3'-O3'	-2.19	1.53	1.60
2	A	999	YE1	P3'-O3'	-2.16	1.53	1.60
2	C	999	YE1	P3'-O3'	-2.14	1.53	1.60
2	A	999	YE1	C2A-N1A	2.09	1.37	1.33
2	C	999	YE1	C2A-N1A	2.10	1.37	1.33
2	B	999	YE1	C2A-N1A	2.12	1.37	1.33
2	A	999	YE1	C5P-N4P	2.90	1.40	1.33
2	B	999	YE1	C5P-N4P	2.90	1.40	1.33
2	C	999	YE1	C5P-N4P	2.92	1.40	1.33
2	C	999	YE1	CAB-NAA	2.96	1.40	1.33
2	B	999	YE1	CAB-NAA	2.96	1.40	1.33
2	A	999	YE1	CAB-NAA	2.98	1.40	1.33
2	A	999	YE1	C9P-N8P	3.23	1.40	1.33
2	B	999	YE1	C9P-N8P	3.24	1.40	1.33
2	C	999	YE1	C9P-N8P	3.26	1.40	1.33
2	A	999	YE1	OAD-CAB	9.15	1.42	1.23
2	B	999	YE1	OAD-CAB	9.16	1.42	1.23
2	C	999	YE1	OAD-CAB	9.19	1.42	1.23

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	999	YE1	C2P-NAA-CAB	-6.93	109.15	122.79
2	B	999	YE1	C2P-NAA-CAB	-6.93	109.15	122.79
2	A	999	YE1	C2P-NAA-CAB	-6.93	109.17	122.79
2	C	999	YE1	C3P-N4P-C5P	-6.77	109.47	122.79
2	A	999	YE1	C3P-N4P-C5P	-6.77	109.47	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	999	YE1	C3P-N4P-C5P	-6.75	109.51	122.79
2	B	999	YE1	C7P-N8P-C9P	-6.55	109.57	122.53
2	A	999	YE1	C7P-N8P-C9P	-6.54	109.58	122.53
2	C	999	YE1	C7P-N8P-C9P	-6.54	109.59	122.53
2	A	999	YE1	C6P-C7P-N8P	-6.25	98.17	111.88
2	B	999	YE1	C6P-C7P-N8P	-6.24	98.18	111.88
2	C	999	YE1	C6P-C7P-N8P	-6.22	98.23	111.88
2	B	999	YE1	C2'-C1'-N9A	-5.31	106.18	114.29
2	A	999	YE1	C2'-C1'-N9A	-5.31	106.18	114.29
2	C	999	YE1	C2'-C1'-N9A	-5.29	106.21	114.29
2	C	999	YE1	P3'-O3'-C3'	-5.08	109.38	121.56
2	B	999	YE1	P3'-O3'-C3'	-5.08	109.38	121.56
2	A	999	YE1	P3'-O3'-C3'	-5.07	109.40	121.56
2	A	999	YE1	O4A-P2A-O6A	-4.83	84.10	108.46
2	B	999	YE1	O4A-P2A-O6A	-4.82	84.13	108.46
2	C	999	YE1	O4A-P2A-O6A	-4.82	84.17	108.46
2	A	999	YE1	C7P-C6P-C5P	-4.67	104.61	112.31
2	B	999	YE1	C7P-C6P-C5P	-4.66	104.62	112.31
2	C	999	YE1	C7P-C6P-C5P	-4.65	104.64	112.31
2	B	999	YE1	P2A-O3A-P1A	-2.58	125.50	132.73
2	A	999	YE1	P2A-O3A-P1A	-2.57	125.53	132.73
2	A	999	YE1	O9P-C9P-N8P	-2.56	117.95	123.08
2	B	999	YE1	O9P-C9P-N8P	-2.56	117.95	123.08
2	C	999	YE1	P2A-O3A-P1A	-2.55	125.56	132.73
2	C	999	YE1	O9P-C9P-N8P	-2.55	117.97	123.08
2	B	999	YE1	O3A-P1A-O5'	-2.36	96.68	102.94
2	A	999	YE1	O3A-P1A-O5'	-2.35	96.70	102.94
2	C	999	YE1	O3A-P1A-O5'	-2.33	96.75	102.94
2	A	999	YE1	C13-C11-C12	-2.16	105.71	108.50
2	B	999	YE1	C13-C11-C12	-2.15	105.72	108.50
2	C	999	YE1	C13-C11-C12	-2.14	105.73	108.50
2	B	999	YE1	N3A-C2A-N1A	-2.05	127.32	128.89
2	C	999	YE1	N3A-C2A-N1A	-2.05	127.32	128.89
2	A	999	YE1	N3A-C2A-N1A	-2.04	127.33	128.89
2	C	999	YE1	O1A-P1A-O3A	2.40	115.97	105.09
2	A	999	YE1	O1A-P1A-O3A	2.41	116.01	105.09
2	B	999	YE1	O1A-P1A-O3A	2.41	116.02	105.09
2	A	999	YE1	C4A-C5A-N7A	2.51	111.79	109.48
2	C	999	YE1	C4A-C5A-N7A	2.55	111.83	109.48
2	B	999	YE1	C4A-C5A-N7A	2.57	111.84	109.48
2	C	999	YE1	C14-C11-C10	2.66	114.20	109.34
2	B	999	YE1	C14-C11-C10	2.69	114.25	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	999	YE1	C14-C11-C10	2.69	114.26	109.34
2	B	999	YE1	O3A-P2A-O6A	3.21	111.45	102.94
2	C	999	YE1	O3A-P2A-O6A	3.21	111.46	102.94
2	A	999	YE1	O3A-P2A-O6A	3.22	111.48	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	YE1	10	0
2	B	999	YE1	8	0
2	C	999	YE1	9	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, 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(Å²)	Q<0.9
1	A	423/440 (96%)	0.10	19 (4%)	37 40	17, 35, 61, 71	0
1	B	422/440 (95%)	-0.10	3 (0%)	89 90	17, 34, 52, 61	0
1	C	421/440 (95%)	0.00	10 (2%)	62 65	16, 33, 57, 68	0
All	All	1266/1320 (95%)	-0.00	32 (2%)	61 63	16, 34, 55, 71	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ALA	5.7
1	A	11	THR	4.8
1	A	43	ARG	4.3
1	A	32	LEU	3.7
1	C	101	GLN	3.6
1	B	107	ARG	3.6
1	C	34	GLU	3.3
1	A	34	GLU	3.1
1	A	30	ALA	3.0
1	A	31	THR	2.9
1	C	13	GLY	2.9
1	A	35	HIS	2.9
1	C	37	ALA	2.9
1	C	31	THR	2.8
1	A	101	GLN	2.7
1	C	26	GLU	2.7
1	A	75	HIS	2.6
1	B	270	ASP	2.6
1	A	38	ARG	2.5
1	A	36	GLY	2.5
1	A	71	ARG	2.5
1	C	29	LEU	2.5
1	C	20	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	29	LEU	2.3
1	C	315	PHE	2.3
1	B	78	VAL	2.3
1	A	42	GLU	2.2
1	A	40	SER	2.2
1	A	228	LYS	2.2
1	A	67	ALA	2.1
1	A	226	ARG	2.0
1	C	23	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	OXY	C	888	2/2	0.79	0.31	12.92	55,55,55,55	0
2	YE1	A	999	59/59	0.86	0.19	1.74	26,39,78,96	0
2	YE1	C	999	59/59	0.90	0.17	0.63	18,36,66,80	0
2	YE1	B	999	59/59	0.89	0.16	0.41	17,45,68,84	0
3	OXY	A	888	2/2	0.94	0.17	-	49,49,49,49	0
3	OXY	B	888	2/2	0.94	0.18	-	44,44,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.