



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 06:34 PM EDT

PDB ID : 3UM8  
Title : Wild-type Plasmodium falciparum DHFR-TS complexed with cycloguanil and NADPH  
Authors : Vanichtanankul, J.; Chitnumsub, P.; Kamchonwongpaisan, S.; Yuthavong, Y.  
Deposited on : unknown  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

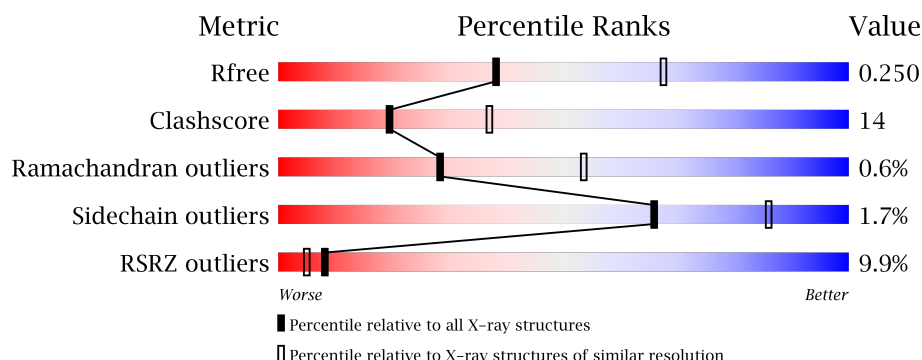
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	608	<div> <div>7%</div> <div>63%</div> <div>26%</div> <div>10%</div> </div>
1	B	608	<div> <div>11%</div> <div>62%</div> <div>25%</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

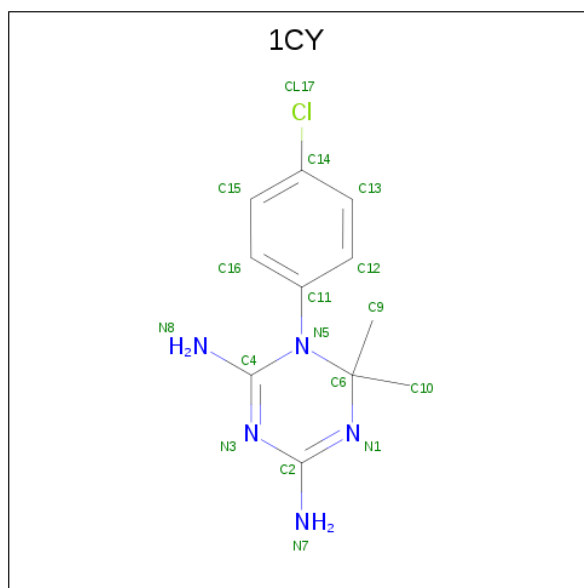
There are 5 unique types of molecules in this entry. The entry contains 9640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4543	2931	750	834	28			
1	B	542	Total	C	N	O	S	0	0	0
			4501	2906	742	825	28			

- Molecule 2 is 1-(4-chlorophenyl)-6,6-dimethyl-1,6-dihydro-1,3,5-triazine-2,4-diamine (three-letter code: 1CY) (formula: C<sub>11</sub>H<sub>14</sub>ClN<sub>5</sub>).



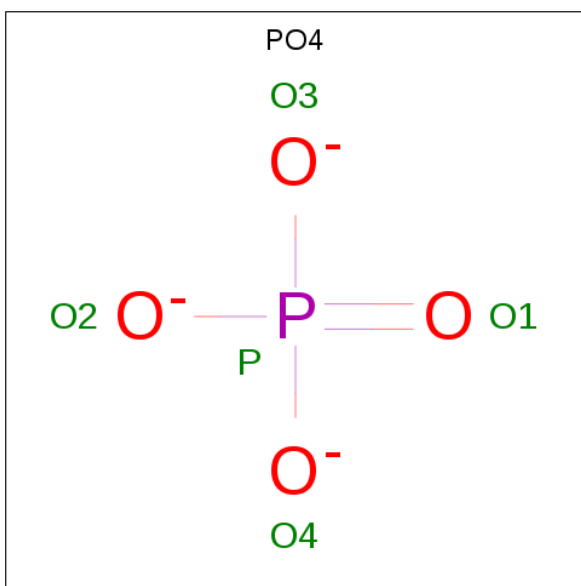
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	B	1	Total	C	Cl	N	0	0
			17	11	1	5		

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



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0

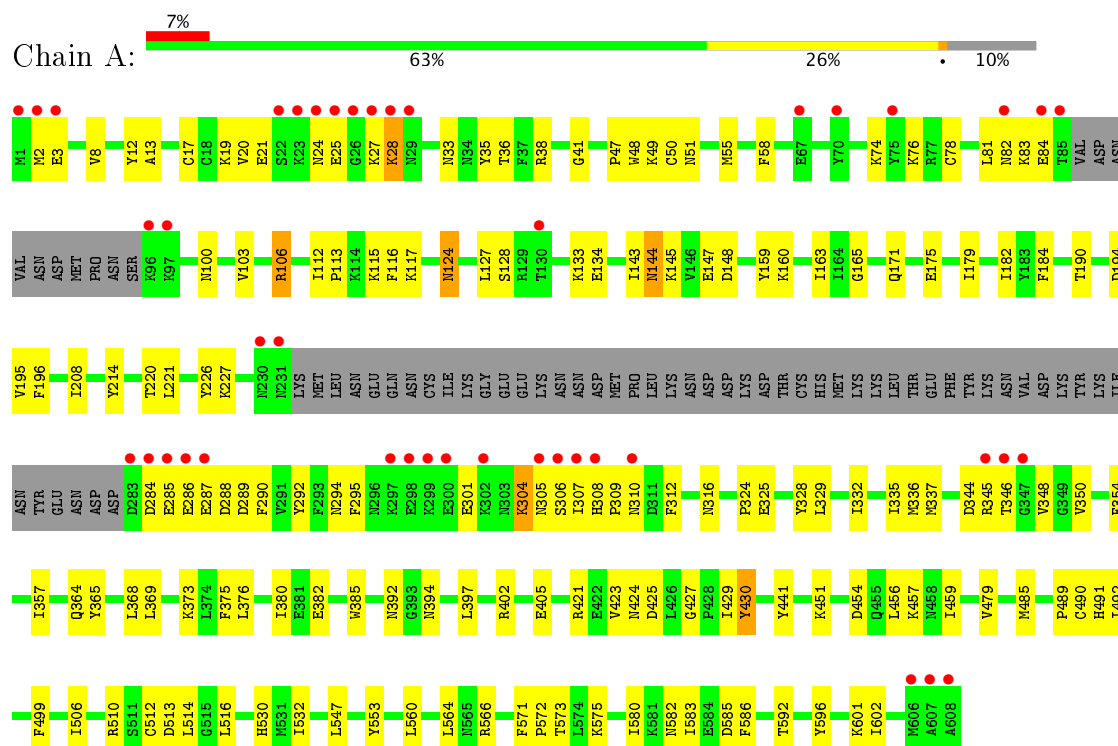
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total 250	O 250	0	0
5	B	206	Total 206	O 206	0	0

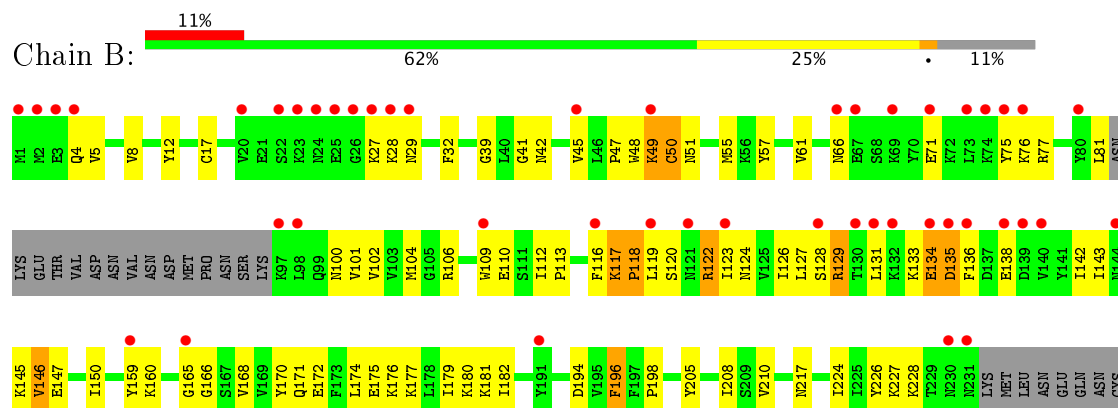
### 3 Residue-property plots

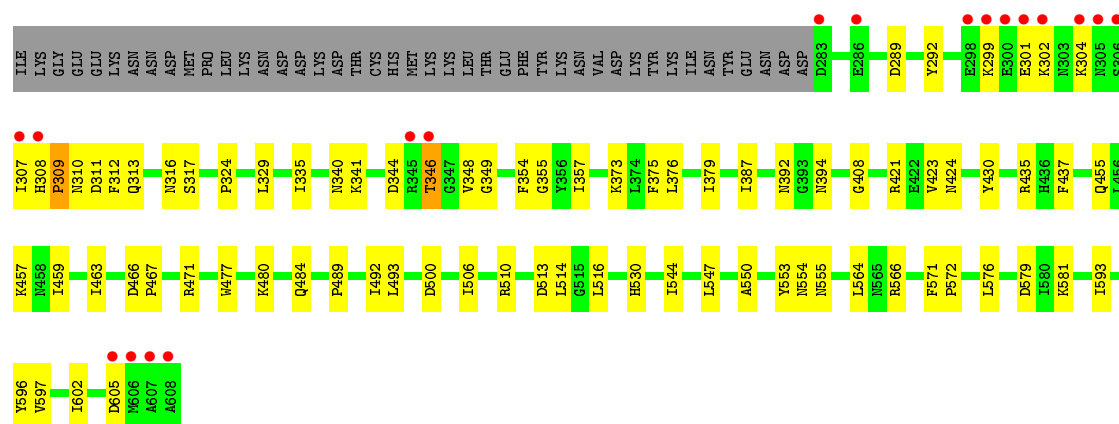
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.76 Å 157.54 Å 164.51 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.60 38.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.16-2.60) 98.4 (38.09-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.212 , 0.258 0.208 , 0.250	Depositor DCC
$R_{free}$ test set	2366 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 1CY, PO4

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	0.41	1/4648 (0.0%)	0.63	0/6272
1	B	0.44	2/4606 (0.0%)	0.63	0/6217
All	All	0.42	3/9254 (0.0%)	0.63	0/12489

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	LYS	C-N	-6.50	1.21	1.34
1	A	286	GLU	CB-CG	6.21	1.64	1.52
1	B	118	PRO	CG-CD	5.47	1.68	1.50

There are no bond angle outliers.

There are no chirality outliers.

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	4543	0	4497	129	0
1	B	4501	0	4452	140	0
2	A	17	0	14	1	0
2	B	17	0	14	0	0
3	A	48	0	26	3	0
3	B	48	0	26	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	1	0
5	A	250	0	0	5	0
5	B	206	0	0	8	0
All	All	9640	0	9029	263	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 14.

All (263) 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:B:376:LEU:HD22	1:B:379:ILE:HD11	1.41	1.00
1:B:102:VAL:HG22	1:B:123:ILE:O	1.64	0.97
1:B:145:LYS:HG2	1:B:146:VAL:H	1.28	0.97
1:B:119:LEU:HB3	1:B:122:ARG:CZ	1.95	0.96
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.53	0.90
1:A:165:GLY:HA3	3:A:610:NDP:H5N	1.57	0.86
1:A:451:LYS:NZ	5:A:1450:HOH:O	2.11	0.83
1:B:101:VAL:HA	1:B:123:ILE:HB	1.61	0.82
1:B:165:GLY:HA3	3:B:710:NDP:H5N	1.59	0.81
1:B:51:ASN:O	1:B:55:MET:HG2	1.83	0.79
1:A:50:CYS:HA	1:A:55:MET:HE1	1.64	0.79
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.65	0.78
1:A:51:ASN:H	1:A:55:MET:CE	1.99	0.76
1:A:346:THR:O	1:A:346:THR:HG22	1.83	0.76
1:A:28:LYS:HA	1:A:28:LYS:NZ	2.01	0.75
1:B:329:LEU:HD22	1:B:564:LEU:HD23	1.69	0.75
1:A:20:VAL:HG12	1:A:21:GLU:N	2.01	0.75
1:B:301:GLU:HB2	1:B:304:LYS:HB2	1.67	0.75
1:B:29:ASN:HB3	1:B:32:PHE:CZ	2.21	0.75
1:B:102:VAL:CG2	1:B:123:ILE:O	2.35	0.73
1:A:301:GLU:O	1:A:304:LYS:HD2	1.87	0.73
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.72	0.72
1:B:100:ASN:O	1:B:123:ILE:HB	1.90	0.72
1:B:145:LYS:HG2	1:B:146:VAL:N	2.03	0.72
1:A:78:CYS:HB3	1:A:83:LYS:O	1.90	0.71
1:A:28:LYS:HA	1:A:28:LYS:HZ3	1.54	0.71
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.72	0.70
1:A:106:ARG:HG3	3:A:610:NDP:O3X	1.91	0.70
1:B:120:SER:N	1:B:122:ARG:HH21	1.89	0.70
1:A:124:ASN:N	1:A:124:ASN:HD22	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASN:O	1:A:27:LYS:HG2	1.92	0.69
1:B:5:VAL:HG11	1:B:150:ILE:HD12	1.72	0.69
1:B:335:ILE:HD12	1:B:514:LEU:HD13	1.74	0.69
1:A:304:LYS:HD3	1:A:305:ASN:N	2.08	0.68
1:B:119:LEU:HB3	1:B:122:ARG:NH2	2.09	0.68
1:B:344:ASP:HB3	1:B:348:VAL:O	1.94	0.68
1:A:112:ILE:O	1:A:117:LYS:HE3	1.93	0.68
1:A:51:ASN:H	1:A:55:MET:HE3	1.59	0.67
1:B:104:MET:HA	1:B:165:GLY:O	1.93	0.67
1:A:491:HIS:CE1	5:A:1413:HOH:O	2.46	0.67
1:A:106:ARG:HH11	1:A:106:ARG:HG3	1.60	0.67
1:A:194:ASP:OD1	1:A:195:VAL:HG23	1.95	0.67
1:A:20:VAL:CG1	1:A:21:GLU:N	2.58	0.67
1:B:126:ILE:N	1:B:126:ILE:HD12	2.10	0.66
1:B:500:ASP:O	5:B:1433:HOH:O	2.13	0.66
1:B:471:ARG:NH1	5:B:1334:HOH:O	2.26	0.66
1:A:165:GLY:HA3	3:A:610:NDP:C5N	2.27	0.65
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.79	0.65
1:B:136:PHE:CD1	1:B:142:ILE:HD11	2.32	0.65
1:A:21:GLU:HG2	1:A:21:GLU:O	1.97	0.64
1:A:304:LYS:HD3	1:A:305:ASN:H	1.61	0.64
1:A:145:LYS:HG2	1:A:148:ASP:OD2	1.98	0.64
1:A:304:LYS:HD2	1:A:304:LYS:H	1.64	0.63
1:B:492:ILE:HD11	1:B:510:ARG:HD3	1.81	0.63
1:B:106:ARG:O	1:B:110:GLU:HG3	1.99	0.62
1:A:147:GLU:H	1:A:147:GLU:CD	2.04	0.61
1:B:346:THR:HG22	1:B:348:VAL:HG22	1.82	0.60
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.35	0.60
1:B:29:ASN:HB3	1:B:32:PHE:CE1	2.36	0.60
1:B:131:LEU:HD22	1:B:136:PHE:CE1	2.37	0.60
1:B:27:LYS:HG3	1:B:28:LYS:N	2.17	0.59
1:B:346:THR:CG2	1:B:348:VAL:HG22	2.33	0.59
1:B:179:ILE:HB	1:B:205:TYR:OH	2.03	0.59
1:A:285:GLU:OE2	1:B:160:LYS:NZ	2.30	0.59
1:B:166:GLY:HA2	3:B:710:NDP:H5N	1.85	0.59
1:B:50:CYS:O	1:B:217:ASN:ND2	2.36	0.58
1:A:12:TYR:CE2	1:A:160:LYS:HD3	2.39	0.58
1:A:27:LYS:O	1:A:27:LYS:HG3	2.02	0.58
1:B:133:LYS:HD2	1:B:133:LYS:H	1.67	0.58
1:B:127:LEU:HA	1:B:143:ILE:HG13	1.84	0.58
1:B:42:ASN:HA	1:B:194:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:ASP:O	1:B:581:LYS:HG2	2.05	0.57
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.05	0.56
1:B:373:LYS:HE2	1:B:375:PHE:CE1	2.40	0.56
1:A:51:ASN:H	1:A:55:MET:HE1	1.70	0.56
1:A:306:SER:O	1:A:307:ILE:HD13	2.06	0.56
1:B:109:TRP:O	1:B:117:LYS:HE2	2.05	0.56
1:A:345:ARG:O	1:A:346:THR:HB	2.06	0.56
1:A:289:ASP:HA	1:A:292:TYR:CD2	2.40	0.56
1:A:214:TYR:O	1:A:220:THR:HA	2.06	0.55
1:A:506:ILE:HG13	1:B:354:PHE:CE2	2.41	0.55
1:B:118:PRO:HB2	1:B:124:ASN:ND2	2.21	0.55
1:B:166:GLY:HA2	3:B:710:NDP:C5N	2.37	0.55
1:A:13:ALA:HB2	1:A:179:ILE:HD12	1.89	0.55
1:B:302:LYS:HZ3	1:B:341:LYS:H	1.54	0.55
1:A:485:MET:SD	1:A:489:PRO:HD3	2.47	0.55
1:B:168:VAL:O	1:B:172:GLU:HG2	2.06	0.55
1:B:553:TYR:HB3	1:B:555:ASN:OD1	2.07	0.55
1:A:159:TYR:CD2	1:A:160:LYS:HG3	2.42	0.55
1:A:329:LEU:HD22	1:A:564:LEU:HD23	1.88	0.54
1:B:457:LYS:HB3	1:B:457:LYS:NZ	2.23	0.54
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.42	0.54
1:A:376:LEU:O	1:A:380:ILE:HG13	2.07	0.54
1:B:48:TRP:O	1:B:49:LYS:HB3	2.07	0.54
1:B:109:TRP:CE2	1:B:117:LYS:HD3	2.42	0.54
1:A:81:LEU:O	1:A:82:ASN:HB2	2.08	0.54
1:A:301:GLU:OE1	1:A:337:MET:HB3	2.08	0.53
1:A:324:PRO:HB2	1:A:571:PHE:HE2	1.73	0.53
1:B:208:ILE:HD13	1:B:227:LYS:HB2	1.89	0.53
1:B:308:HIS:HB2	1:B:311:ASP:OD1	2.08	0.53
1:B:168:VAL:HG23	3:B:710:NDP:O1N	2.07	0.53
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.44	0.53
1:A:513:ASP:OD2	1:A:516:LEU:HB2	2.08	0.53
1:A:368:LEU:HD13	1:A:376:LEU:HD11	1.90	0.53
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.91	0.52
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.09	0.52
1:B:120:SER:O	1:B:122:ARG:NH2	2.42	0.52
1:B:547:LEU:HD12	1:B:547:LEU:N	2.25	0.52
1:B:210:VAL:HG12	1:B:224:ILE:CG2	2.39	0.52
1:B:109:TRP:CZ2	1:B:117:LYS:HD3	2.45	0.52
1:A:490:CYS:SG	5:A:1303:HOH:O	2.59	0.52
1:B:172:GLU:O	1:B:176:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:O	1:B:463:ILE:HG13	2.10	0.52
1:B:133:LYS:CD	1:B:133:LYS:H	2.22	0.52
1:B:102:VAL:HG21	1:B:122:ARG:HG2	1.93	0.51
1:B:477:TRP:HE3	1:B:489:PRO:HG2	1.75	0.51
1:A:2:MET:HG2	1:A:3:GLU:N	2.26	0.51
1:A:332:ILE:HD13	1:A:560:LEU:HD22	1.93	0.51
1:A:335:ILE:HD12	1:A:514:LEU:HD13	1.93	0.51
1:B:376:LEU:CD2	1:B:379:ILE:HD11	2.26	0.51
1:B:4:GLN:O	1:B:8:VAL:HG23	2.10	0.51
1:B:572:PRO:HB3	1:B:596:TYR:HA	1.92	0.51
1:B:349:GLY:C	1:B:554:ASN:ND2	2.64	0.51
1:A:171:GLN:O	1:A:175:GLU:HB2	2.10	0.50
1:A:382:GLU:O	1:A:385:TRP:HB3	2.11	0.50
1:B:480:LYS:HE2	5:B:1233:HOH:O	2.11	0.50
1:B:324:PRO:HB2	1:B:571:PHE:HE2	1.76	0.50
1:A:304:LYS:HD2	1:A:304:LYS:N	2.27	0.50
1:A:344:ASP:HB3	1:A:348:VAL:HB	1.94	0.50
1:A:373:LYS:HB3	1:A:601:LYS:HB3	1.94	0.50
1:B:48:TRP:O	1:B:49:LYS:CB	2.59	0.50
1:A:423:VAL:O	1:A:424:ASN:HB2	2.11	0.50
1:B:493:LEU:HD12	1:B:493:LEU:C	2.32	0.49
1:A:115:LYS:HE3	1:A:116:PHE:CE2	2.48	0.49
1:A:582:ASN:HB3	1:A:585:ASP:OD2	2.11	0.49
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.94	0.49
1:A:392:ASN:OD1	1:A:394:ASN:HB2	2.13	0.49
1:A:530:HIS:CE1	5:A:1434:HOH:O	2.66	0.49
1:B:133:LYS:N	1:B:133:LYS:HD2	2.28	0.49
1:A:456:LEU:O	1:A:459:ILE:HG13	2.13	0.49
1:A:124:ASN:N	1:A:124:ASN:ND2	2.60	0.49
1:A:19:LYS:O	1:A:190:THR:HA	2.13	0.49
1:A:50:CYS:CA	1:A:55:MET:HE1	2.40	0.49
1:B:530:HIS:HB3	1:B:576:LEU:HD11	1.94	0.49
1:A:33:ASN:H	1:A:36:THR:HG1	1.61	0.48
1:A:421:ARG:HD2	1:A:425:ASP:CG	2.34	0.48
1:B:457:LYS:HB3	1:B:457:LYS:HZ2	1.78	0.48
1:A:346:THR:O	1:A:346:THR:CG2	2.55	0.48
1:A:421:ARG:HH11	1:A:421:ARG:HG2	1.79	0.48
1:B:47:PRO:HB2	1:B:48:TRP:CE3	2.49	0.48
1:B:376:LEU:HD12	1:B:593:ILE:HG13	1.96	0.48
1:A:58:PHE:CZ	2:A:609:1CY:H16	2.49	0.47
1:B:307:ILE:CG2	1:B:312:PHE:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CE1	1:A:294:ASN:ND2	2.82	0.47
1:B:171:GLN:HA	1:B:198:PRO:HG2	1.96	0.47
1:B:423:VAL:O	1:B:424:ASN:HB2	2.14	0.47
1:B:109:TRP:CH2	1:B:118:PRO:HB3	2.49	0.47
1:B:113:PRO:HG2	1:B:116:PHE:HD2	1.79	0.47
1:A:128:SER:O	1:A:144:ASN:HA	2.14	0.47
1:A:290:PHE:O	1:A:294:ASN:ND2	2.46	0.47
1:B:12:TYR:CE1	1:B:180:LYS:HD3	2.49	0.47
1:B:355:GLY:HA2	1:B:547:LEU:O	2.15	0.47
1:A:159:TYR:CE2	1:A:160:LYS:HE3	2.49	0.47
1:A:532:ILE:HD13	1:A:583:ILE:HD13	1.96	0.47
1:A:575:LYS:HB2	1:A:592:THR:HB	1.96	0.47
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.80	0.47
1:B:32:PHE:CD1	1:B:597:VAL:HG13	2.50	0.47
1:B:312:PHE:HB2	1:B:316:ASN:HD22	1.80	0.47
1:A:20:VAL:HG21	1:A:196:PHE:HE1	1.80	0.46
1:B:17:CYS:HA	1:B:39:GLY:O	2.15	0.46
1:A:144:ASN:HD21	1:A:145:LYS:NZ	2.14	0.46
1:B:129:ARG:HG3	3:B:710:NDP:O1X	2.16	0.46
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.51	0.46
1:B:75:TYR:HD1	1:B:76:LYS:HG3	1.80	0.46
1:A:103:VAL:HB	1:A:163:ILE:HD13	1.96	0.46
1:A:17:CYS:HB2	1:A:184:PHE:CE1	2.49	0.46
1:B:313:GLN:O	1:B:317:SER:HB3	2.16	0.46
1:B:566:ARG:NH1	1:B:602:ILE:HD11	2.30	0.46
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.31	0.46
1:A:20:VAL:HG21	1:A:196:PHE:CE1	2.51	0.46
1:B:102:VAL:CG2	1:B:122:ARG:HG2	2.46	0.46
1:B:120:SER:N	1:B:122:ARG:NH2	2.60	0.46
1:B:455:GLN:HA	5:B:1420:HOH:O	2.16	0.45
1:B:45:VAL:HB	5:B:1362:HOH:O	2.16	0.45
1:A:20:VAL:CG1	1:A:21:GLU:H	2.27	0.45
1:A:83:LYS:O	1:A:84:GLU:HG3	2.17	0.45
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.99	0.45
1:B:112:ILE:HB	1:B:117:LYS:HE2	1.98	0.45
1:B:307:ILE:HG22	1:B:307:ILE:O	2.16	0.44
1:B:484:GLN:HG3	5:B:1161:HOH:O	2.16	0.44
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.51	0.44
1:A:301:GLU:O	1:A:304:LYS:CD	2.62	0.44
1:A:304:LYS:N	1:A:304:LYS:CD	2.80	0.44
1:B:134:GLU:N	1:B:134:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TRP:O	1:A:49:LYS:HB2	2.16	0.44
1:B:5:VAL:O	1:B:8:VAL:N	2.46	0.44
1:A:106:ARG:CG	1:A:106:ARG:HH11	2.29	0.44
1:A:325:GLU:HG3	1:A:369:LEU:HD22	2.00	0.44
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.52	0.44
1:B:127:LEU:O	3:B:710:NDP:H1B	2.18	0.44
1:B:310:ASN:O	1:B:310:ASN:ND2	2.51	0.44
1:A:144:ASN:HD21	1:A:145:LYS:HZ2	1.66	0.44
1:B:131:LEU:HD22	1:B:136:PHE:CZ	2.53	0.44
1:A:208:ILE:HD13	1:A:227:LYS:HB2	2.00	0.44
1:B:101:VAL:HG22	1:B:123:ILE:HG21	2.00	0.44
1:A:113:PRO:HB2	1:A:116:PHE:HD2	1.83	0.43
1:B:101:VAL:HG22	1:B:123:ILE:HD13	1.99	0.43
1:A:572:PRO:HB3	1:A:596:TYR:HA	2.01	0.43
1:B:138:GLU:H	1:B:138:GLU:CD	2.22	0.43
1:A:357:ILE:HB	1:B:357:ILE:HD11	2.01	0.43
1:A:221:LEU:N	1:A:221:LEU:HD23	2.33	0.43
1:B:126:ILE:CD1	1:B:126:ILE:N	2.81	0.43
1:B:71:GLU:HA	1:B:71:GLU:OE1	2.18	0.43
1:A:144:ASN:HD22	1:A:144:ASN:C	2.21	0.43
1:A:427:GLY:HA2	1:A:441:TYR:CE2	2.54	0.43
1:B:205:TYR:CD1	1:B:228:LYS:HA	2.53	0.43
1:B:387:ILE:O	1:B:435:ARG:NH1	2.52	0.43
1:B:196:PHE:CD1	1:B:196:PHE:N	2.86	0.42
1:A:182:ILE:HB	1:A:226:TYR:HB2	2.00	0.42
1:A:373:LYS:HE3	1:A:375:PHE:CZ	2.53	0.42
1:A:510:ARG:NH1	4:A:801:PO4:O2	2.51	0.42
1:B:75:TYR:HD1	1:B:76:LYS:CG	2.32	0.42
1:A:335:ILE:HD12	1:A:514:LEU:CD1	2.48	0.42
1:A:573:THR:HA	5:A:1159:HOH:O	2.18	0.42
1:B:309:PRO:C	1:B:311:ASP:H	2.22	0.42
1:B:57:TYR:O	1:B:61:VAL:HG23	2.19	0.42
1:A:336:MET:HE3	1:A:560:LEU:HB2	2.01	0.42
1:B:170:TYR:O	1:B:174:LEU:HG	2.20	0.42
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.85	0.42
1:B:466:ASP:N	1:B:467:PRO:CD	2.83	0.42
1:A:454:ASP:OD2	1:A:457:LYS:HD2	2.20	0.42
1:B:175:GLU:O	1:B:177:LYS:HG3	2.20	0.42
1:B:112:ILE:O	1:B:117:LYS:HE3	2.20	0.42
1:B:308:HIS:HB3	1:B:309:PRO:HD2	2.01	0.42
1:A:35:TYR:O	1:A:38:ARG:NH1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ASP:OD2	1:B:516:LEU:HB3	2.19	0.41
1:B:77:ARG:O	1:B:81:LEU:HG	2.19	0.41
1:A:147:GLU:CD	1:A:147:GLU:N	2.72	0.41
1:A:429:ILE:O	1:A:430:TYR:C	2.58	0.41
1:B:514:LEU:HD11	1:B:550:ALA:HB1	2.02	0.41
1:A:397:LEU:HD22	1:A:402:ARG:NH1	2.35	0.41
1:B:392:ASN:OD1	1:B:394:ASN:HB2	2.20	0.41
1:A:312:PHE:HB2	1:A:316:ASN:ND2	2.36	0.41
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.60	0.41
1:B:134:GLU:O	1:B:135:ASP:C	2.58	0.41
1:A:74:LYS:O	1:A:78:CYS:HB2	2.21	0.41
1:B:572:PRO:HD3	5:B:1042:HOH:O	2.20	0.41
1:A:292:TYR:O	1:A:295:PHE:HB3	2.21	0.41
1:B:106:ARG:HB2	1:B:128:SER:HB2	2.03	0.41
1:B:289:ASP:HA	1:B:292:TYR:CD2	2.55	0.41
1:B:32:PHE:CG	1:B:597:VAL:HG13	2.56	0.41
1:A:566:ARG:CZ	1:A:602:ILE:HD11	2.51	0.41
1:B:605:ASP:HB3	5:B:1169:HOH:O	2.20	0.41
1:A:308:HIS:HB3	1:A:309:PRO:HD2	2.02	0.41
1:A:364:GLN:O	1:A:365:TYR:HB3	2.20	0.41
1:B:408:GLY:O	1:B:423:VAL:HG13	2.21	0.40
1:A:133:LYS:HE2	1:A:134:GLU:OE2	2.22	0.40
1:B:335:ILE:CD1	1:B:514:LEU:HD13	2.47	0.40
1:A:402:ARG:NH1	1:A:405:GLU:OE2	2.54	0.40
1:A:580:ILE:HG21	1:A:586:PHE:CG	2.56	0.40
1:A:144:ASN:H	1:A:144:ASN:ND2	2.20	0.40
1:B:299:LYS:HD2	1:B:299:LYS:HA	1.88	0.40
1:A:285:GLU:C	1:A:287:GLU:N	2.73	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	541/608 (89%)	503 (93%)	36 (7%)	2 (0%)	38	63
1	B	536/608 (88%)	490 (91%)	42 (8%)	4 (1%)	25	49
All	All	1077/1216 (89%)	993 (92%)	78 (7%)	6 (1%)	28	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	TYR
1	B	49	LYS
1	B	430	TYR
1	A	25	GLU
1	B	309	PRO
1	B	146	VAL

### 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	510/570 (90%)	502 (98%)	8 (2%)	68	87
1	B	505/570 (89%)	496 (98%)	9 (2%)	64	85
All	All	1015/1140 (89%)	998 (98%)	17 (2%)	66	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	106	ARG
1	A	124	ASN
1	A	144	ASN
1	A	284	ASP
1	A	288	ASP
1	A	304	LYS
1	A	310	ASN
1	B	50	CYS
1	B	66	ASN

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Mol	Chain	Res	Type
1	B	122	ARG
1	B	129	ARG
1	B	134	GLU
1	B	135	ASP
1	B	147	GLU
1	B	196	PHE
1	B	346	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	157	ASN
1	A	171	GLN
1	A	201	ASN
1	A	294	ASN
1	A	310	ASN
1	A	316	ASN
1	A	394	ASN
1	A	407	ASN
1	A	424	ASN
1	B	4	GLN
1	B	24	ASN
1	B	66	ASN
1	B	99	GLN
1	B	310	ASN
1	B	313	GLN
1	B	316	ASN
1	B	394	ASN
1	B	424	ASN
1	B	530	HIS
1	B	554	ASN
1	B	582	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
2	1CY	A	609	-	15,18,18	3.45	10 (66%)	17,27,27	1.15	1 (5%)
3	NDP	A	610	-	43,52,52	1.32	4 (9%)	49,80,80	2.12	9 (18%)
4	PO4	A	801	-	4,4,4	1.44	0	6,6,6	0.39	0
4	PO4	A	802	-	4,4,4	1.45	0	6,6,6	0.39	0
2	1CY	B	709	-	15,18,18	3.40	10 (66%)	17,27,27	1.41	2 (11%)
3	NDP	B	710	-	43,52,52	1.38	5 (11%)	49,80,80	2.14	7 (14%)

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	1CY	A	609	-	-	0/4/23/23	0/2/2/2
3	NDP	A	610	-	-	0/30/77/77	0/5/5/5
4	PO4	A	801	-	-	0/0/0/0	0/0/0/0
4	PO4	A	802	-	-	0/0/0/0	0/0/0/0
2	1CY	B	709	-	-	0/4/23/23	0/2/2/2
3	NDP	B	710	-	-	0/30/77/77	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	609	1CY	C14-CL17	-4.83	1.64	1.74
2	B	709	1CY	C14-CL17	-2.65	1.68	1.74
3	A	610	NDP	C5D-C4D	2.00	1.57	1.51
3	B	710	NDP	O4D-C1D	2.10	1.47	1.42
3	A	610	NDP	O4D-C1D	2.18	1.47	1.42
3	B	710	NDP	C8A-N7A	2.23	1.38	1.34
3	B	710	NDP	C5D-C4D	2.38	1.59	1.51
2	A	609	1CY	C4-N8	2.40	1.38	1.34
2	A	609	1CY	C12-C13	2.68	1.43	1.38
3	B	710	NDP	C4A-N3A	2.74	1.39	1.35
2	A	609	1CY	C16-C15	2.93	1.44	1.38
2	B	709	1CY	C12-C13	2.94	1.44	1.38
3	A	610	NDP	C4A-N3A	2.94	1.39	1.35
2	B	709	1CY	C2-N7	2.98	1.41	1.34
2	A	609	1CY	C2-N7	3.09	1.42	1.34
2	A	609	1CY	C13-C14	3.21	1.44	1.38
2	B	709	1CY	C4-N8	3.49	1.40	1.34
2	B	709	1CY	C13-C14	3.89	1.45	1.38
2	B	709	1CY	C12-C11	3.89	1.47	1.39
3	A	610	NDP	C6N-N1N	4.09	1.48	1.37
2	A	609	1CY	C12-C11	4.13	1.47	1.39
3	B	710	NDP	C6N-N1N	4.39	1.49	1.37
2	B	709	1CY	C2-N3	4.48	1.44	1.36
2	A	609	1CY	C2-N3	4.49	1.44	1.36
2	B	709	1CY	C16-C15	4.55	1.46	1.38
2	B	709	1CY	C15-C14	5.23	1.48	1.38
2	A	609	1CY	C15-C14	5.41	1.48	1.38
2	B	709	1CY	C16-C11	5.73	1.51	1.39
2	A	609	1CY	C16-C11	6.29	1.52	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	710	NDP	N3A-C2A-N1A	-11.40	118.93	128.86
3	A	610	NDP	N3A-C2A-N1A	-10.47	119.74	128.86
3	A	610	NDP	C1D-N1N-C2N	-4.51	113.43	121.09
2	B	709	1CY	C9-C6-C10	-4.16	104.75	110.90
3	B	710	NDP	C1B-N9A-C4A	-3.77	120.12	126.64
2	A	609	1CY	C9-C6-C10	-3.72	105.41	110.90
3	B	710	NDP	O4B-C1B-C2B	-3.62	100.26	106.59
3	A	610	NDP	O2B-C2B-C3B	-3.39	99.06	111.63
3	B	710	NDP	O2B-C2B-C3B	-3.14	100.00	111.63
3	A	610	NDP	C1B-N9A-C4A	-3.00	121.45	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	610	NDP	O4B-C1B-C2B	-3.00	101.35	106.59
3	A	610	NDP	C3N-C2N-N1N	-2.12	120.01	123.08
3	B	710	NDP	C3N-C2N-N1N	-2.07	120.08	123.08
3	A	610	NDP	C2D-C1D-N1N	2.22	119.03	113.32
2	B	709	1CY	C16-C11-N5	2.66	123.26	120.07
3	A	610	NDP	C4B-O4B-C1B	2.69	112.64	109.77
3	A	610	NDP	C2A-N1A-C6A	2.85	123.76	118.77
3	B	710	NDP	C2A-N1A-C6A	2.89	123.82	118.77
3	B	710	NDP	C4B-O4B-C1B	3.51	113.50	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	609	1CY	1	0
3	A	610	NDP	3	0
4	A	801	PO4	1	0
3	B	710	NDP	6	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

### 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	547/608 (89%)	0.11	43 (7%)	13 9	23, 42, 90, 91	0
1	B	542/608 (89%)	0.49	65 (11%)	5 3	22, 48, 91, 91	0
All	All	1089/1216 (89%)	0.30	108 (9%)	8 5	22, 44, 91, 91	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LYS	10.9
1	B	26	GLY	10.2
1	B	607	ALA	9.1
1	A	305	ASN	8.9
1	A	608	ALA	8.5
1	A	283	ASP	8.4
1	A	2	MET	7.8
1	B	2	MET	7.8
1	B	307	ILE	7.8
1	B	1	MET	7.6
1	A	1	MET	7.4
1	A	284	ASP	7.0
1	B	608	ALA	6.7
1	A	607	ALA	6.5
1	A	24	ASN	6.1
1	B	230	ASN	6.1
1	A	23	LYS	5.8
1	A	27	LYS	5.8
1	B	3	GLU	5.7
1	A	346	THR	5.7
1	A	26	GLY	5.5
1	B	606	MET	5.5
1	B	75	TYR	5.5
1	B	283	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	29	ASN	5.4
1	A	307	ILE	5.3
1	A	25	GLU	5.3
1	B	28	LYS	5.1
1	B	299	LYS	5.1
1	A	286	GLU	5.0
1	B	300	GLU	4.9
1	B	25	GLU	4.9
1	A	85	THR	4.8
1	B	24	ASN	4.8
1	B	4	GLN	4.6
1	A	298	GLU	4.6
1	A	285	GLU	4.5
1	B	131	LEU	4.3
1	B	144	ASN	4.2
1	B	76	LYS	4.2
1	B	136	PHE	4.1
1	A	75	TYR	4.0
1	B	298	GLU	4.0
1	A	22	SER	4.0
1	A	345	ARG	3.9
1	B	304	LYS	3.8
1	A	96	LYS	3.8
1	A	231	ASN	3.8
1	B	346	THR	3.7
1	A	299	LYS	3.7
1	A	606	MET	3.7
1	B	605	ASP	3.6
1	B	80	TYR	3.6
1	B	74	LYS	3.6
1	A	3	GLU	3.6
1	B	45	VAL	3.5
1	B	138	GLU	3.4
1	A	82	ASN	3.4
1	A	84	GLU	3.4
1	A	28	LYS	3.3
1	A	306	SER	3.3
1	A	300	GLU	3.2
1	B	139	ASP	3.2
1	B	128	SER	3.2
1	B	73	LEU	3.2
1	B	116	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	130	THR	3.1
1	A	347	GLY	3.1
1	B	67	GLU	3.1
1	B	231	ASN	3.1
1	B	134	GLU	3.0
1	B	305	ASN	3.0
1	B	135	ASP	3.0
1	B	302	LYS	2.9
1	A	29	ASN	2.9
1	B	306	SER	2.9
1	B	132	LYS	2.9
1	A	230	ASN	2.9
1	B	23	LYS	2.9
1	B	159	TYR	2.8
1	A	287	GLU	2.7
1	B	121	ASN	2.7
1	B	66	ASN	2.6
1	B	109	TRP	2.6
1	A	97	LYS	2.6
1	B	98	LEU	2.6
1	A	302	LYS	2.6
1	B	123	ILE	2.5
1	B	97	LYS	2.5
1	B	119	LEU	2.5
1	B	165	GLY	2.4
1	A	297	LYS	2.4
1	A	70	TYR	2.3
1	B	71	GLU	2.3
1	B	345	ARG	2.3
1	B	140	VAL	2.2
1	A	67	GLU	2.2
1	B	20	VAL	2.2
1	A	308	HIS	2.2
1	A	310	ASN	2.1
1	B	301	GLU	2.1
1	B	286	GLU	2.1
1	B	308	HIS	2.1
1	B	49	LYS	2.1
1	B	22	SER	2.0
1	B	69	LYS	2.0
1	B	191	TYR	2.0
1	A	130	THR	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1CY	B	709	17/17	0.76	0.34	1.66	83,84,89,90	0
4	PO4	A	802	5/5	0.94	0.20	0.95	63,65,66,67	0
2	1CY	A	609	17/17	0.96	0.20	0.40	27,31,38,44	0
3	NDP	B	710	48/48	0.85	0.27	-0.15	88,90,90,90	0
4	PO4	A	801	5/5	0.96	0.16	-0.54	77,78,78,79	0
3	NDP	A	610	48/48	0.95	0.15	-0.78	47,53,58,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.