Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:04 PM GMT

PDB ID	:	1RY8
Title	:	Prostaglandin F synthase complexed with NADPH and rutin
Authors	:	Komoto, J.; Yamada, T.; Watanabe, K.; Takusagawa, F.
Deposited on	:	2003-12-19
Resolution	:	1.69 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

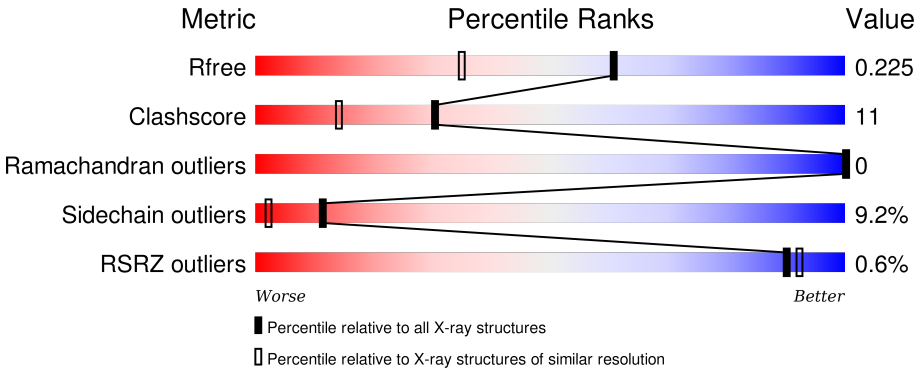
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.69 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	323	% 77% 19%
1	B	323	% 74% 21%

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
2	NDP	A	2324	-	-	-	X

2 Entry composition

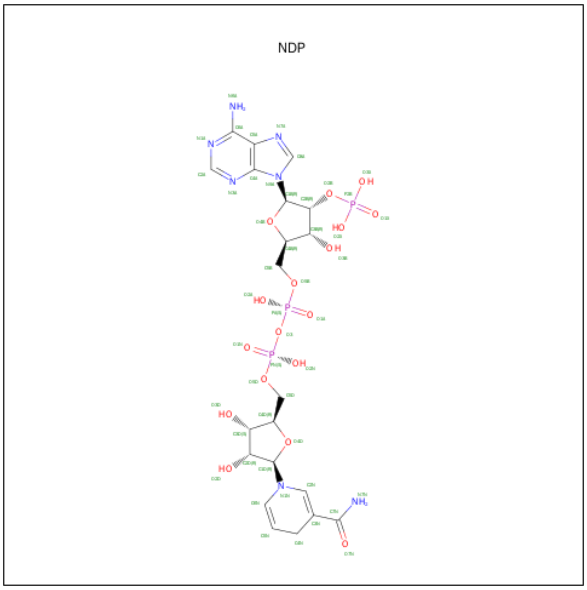
There are 4 unique types of molecules in this entry. The entry contains 5815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldo-keto reductase family 1 member C3.

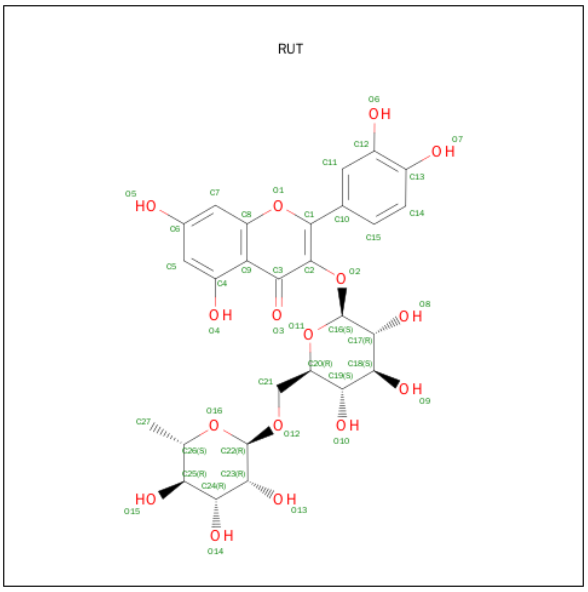
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2563	1632	445	474	12			
1	B	319	Total	C	N	O	S	0	0	0
			2563	1632	445	474	12			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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		

- Molecule 3 is RUTIN (three-letter code: RUT) (formula: $C_{27}H_{30}O_{16}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 43 27 16	0	0
3	B	1	Total C O 43 27 16	0	0

- Molecule 4 is water.

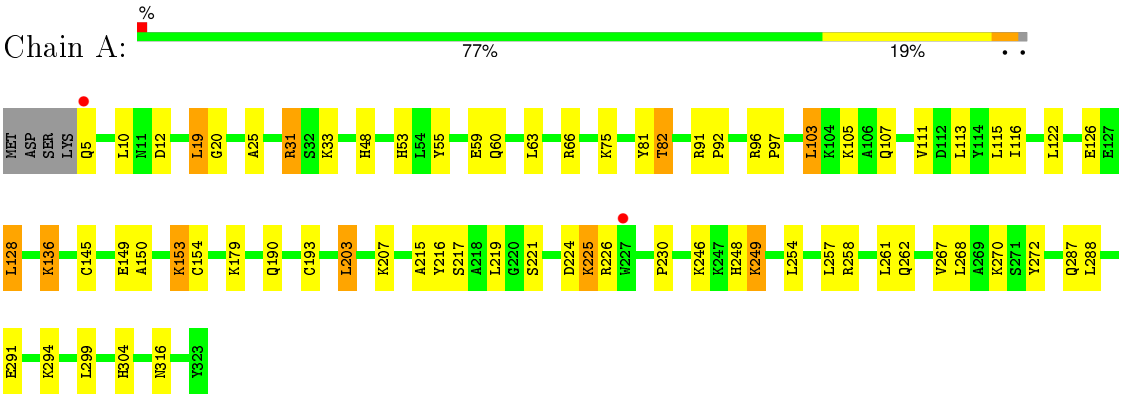
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	253	Total O 253 253	0	0
4	B	254	Total O 254 254	0	0

3 Residue-property plots (i)

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.

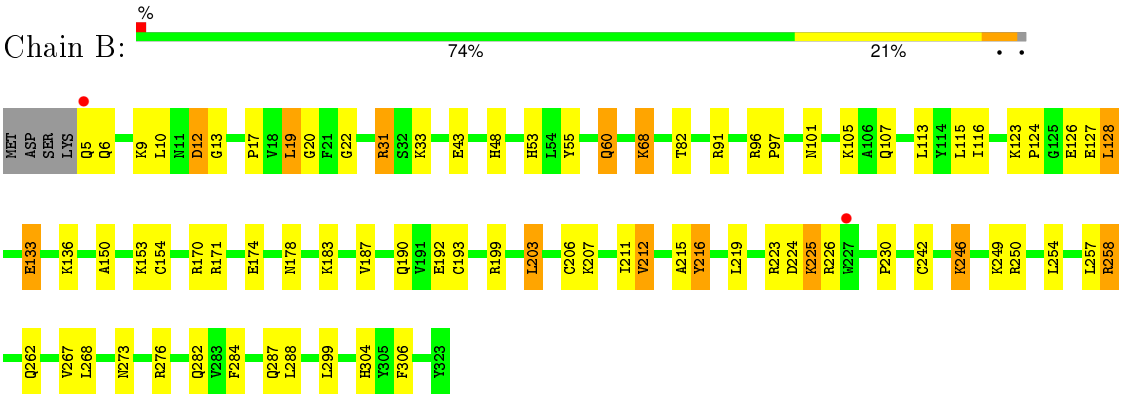
- Molecule 1: Aldo-keto reductase family 1 member C3

Chain A:



- Molecule 1: Aldo-keto reductase family 1 member C3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.06Å 49.37Å 83.59Å 73.90° 86.30° 69.90°	Depositor
Resolution (Å)	10.00 – 1.69 10.99 – 1.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.69) 87.7 (10.99-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.249 0.184 , 0.225	Depositor DCC
R_{free} test set	7306 reflections (10.09%)	DCC
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.15 , 50.7	EDS
Estimated twinning fraction	0.007 for -h,-k,-k+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 72470 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.33	0/2622	0.57	1/3547 (0.0%)
1	B	0.33	0/2622	0.55	1/3547 (0.0%)
All	All	0.33	0/5244	0.56	2/7094 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	ILE	N-CA-C	-5.21	96.92	111.00
1	A	116	ILE	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	216	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2563	0	2558	54	0
1	B	2563	0	2558	57	0
2	A	48	0	26	12	0
2	B	48	0	26	6	0
3	A	43	0	28	1	0
3	B	43	0	28	1	0
4	A	253	0	0	1	0
4	B	254	0	0	2	0
All	All	5815	0	5224	116	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 11.

All (116) 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:262:GLN:HE22	1:B:288:LEU:H	1.04	0.99
1:B:96:ARG:HB2	1:B:153:LYS:HE3	1.43	0.98
1:B:123:LYS:HD2	1:B:124:PRO:HD2	1.52	0.92
1:A:262:GLN:HE22	1:A:288:LEU:H	0.95	0.91
1:A:258:ARG:HE	1:A:262:GLN:HE21	1.20	0.86
1:A:262:GLN:HE22	1:A:288:LEU:N	1.79	0.79
1:B:262:GLN:NE2	1:B:288:LEU:H	1.80	0.78
1:A:262:GLN:NE2	1:A:288:LEU:H	1.79	0.75
1:A:111:VAL:HG12	1:A:113:LEU:H	1.54	0.71
1:B:225:LYS:HD2	1:B:230:PRO:HB3	1.73	0.70
1:B:262:GLN:HE22	1:B:288:LEU:N	1.85	0.69
1:A:150:ALA:HA	1:A:153:LYS:HD3	1.72	0.69
1:B:258:ARG:HD2	1:B:262:GLN:HE21	1.56	0.69
1:A:136:LYS:HA	1:A:136:LYS:HE2	1.76	0.68
1:B:60:GLN:H	1:B:60:GLN:NE2	1.92	0.68
1:A:219:LEU:HB2	2:A:2324:NDP:H52A	1.76	0.67
1:A:10:LEU:C	1:A:12:ASP:H	1.97	0.66
1:B:5:GLN:HA	1:B:284:PHE:CZ	2.31	0.66
1:B:250:ARG:HH11	1:B:282:GLN:HE21	1.43	0.65
1:A:33:LYS:HG2	1:A:272:TYR:HD1	1.61	0.65
1:A:63:LEU:HD23	1:A:66:ARG:NH1	2.13	0.64
1:B:224:ASP:OD1	1:B:226:ARG:HB2	1.97	0.64
1:A:257:LEU:HD23	1:A:267:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:HG3	1:A:179:LYS:HE2	1.81	0.61
1:B:101:ASN:HD21	1:B:105:LYS:HE3	1.65	0.61
1:B:257:LEU:HD13	4:B:1469:HOH:O	2.00	0.60
3:B:3325:RUT:H1	3:B:3325:RUT:O11	2.01	0.60
1:B:216:TYR:CE2	2:B:3324:NDP:H41N	2.35	0.60
3:A:2325:RUT:O11	3:A:2325:RUT:H1	2.01	0.60
1:A:257:LEU:HD23	1:A:267:VAL:CG2	2.32	0.59
1:B:257:LEU:HD23	1:B:267:VAL:HG21	1.83	0.59
1:B:53:HIS:CE1	1:B:128:LEU:HD11	2.38	0.59
1:A:96:ARG:HB2	1:A:153:LYS:HE3	1.84	0.59
1:B:96:ARG:HB2	1:B:153:LYS:CE	2.27	0.58
1:A:225:LYS:HD2	1:A:230:PRO:HB3	1.86	0.56
1:A:33:LYS:HG2	1:A:272:TYR:CD1	2.40	0.56
1:B:153:LYS:HG2	1:B:154:CYS:N	2.21	0.56
1:B:31:ARG:O	1:B:60:GLN:HG2	2.06	0.56
1:B:5:GLN:HA	1:B:284:PHE:CE2	2.41	0.56
1:B:20:GLY:HA2	1:B:48:HIS:HB3	1.88	0.56
1:A:203:LEU:HD22	1:A:207:LYS:HE3	1.88	0.55
1:A:219:LEU:CB	2:A:2324:NDP:H52A	2.36	0.55
1:A:216:TYR:CE2	2:A:2324:NDP:H41N	2.42	0.55
1:A:82:THR:HG21	4:A:1020:HOH:O	2.06	0.54
1:B:242:CYS:O	1:B:246:LYS:HD3	2.07	0.54
1:B:219:LEU:HB2	2:B:3324:NDP:H52A	1.89	0.54
1:B:101:ASN:ND2	1:B:105:LYS:HE3	2.23	0.53
1:B:273:ASN:HB3	1:B:276:ARG:HD3	1.90	0.53
1:B:10:LEU:C	1:B:12:ASP:H	2.10	0.52
1:A:224:ASP:OD1	1:A:226:ARG:HB2	2.10	0.51
1:B:174:GLU:HG3	1:B:178:ASN:ND2	2.25	0.51
1:A:63:LEU:HD23	1:A:66:ARG:HH12	1.75	0.51
1:A:217:SER:H	2:A:2324:NDP:H52N	1.75	0.50
1:B:219:LEU:CB	2:B:3324:NDP:H52A	2.42	0.50
1:B:60:GLN:HE21	1:B:60:GLN:H	1.58	0.50
1:A:10:LEU:C	1:A:12:ASP:N	2.65	0.50
2:A:2324:NDP:H6N	2:A:2324:NDP:H51N	1.92	0.50
1:A:216:TYR:CZ	2:A:2324:NDP:H41N	2.46	0.50
1:A:53:HIS:HE1	1:A:128:LEU:HD11	1.78	0.49
1:B:203:LEU:O	1:B:207:LYS:HG3	2.13	0.49
1:B:9:LYS:HZ2	1:B:13:GLY:HA2	1.78	0.49
1:A:111:VAL:HG12	1:A:113:LEU:N	2.27	0.48
1:A:53:HIS:CE1	1:A:128:LEU:HD11	2.48	0.48
1:B:304:HIS:NE2	1:B:306:PHE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD21	1:A:115:LEU:HD21	1.95	0.48
1:B:5:GLN:HE22	1:B:19:LEU:H	1.60	0.48
1:B:192:GLU:HB2	1:B:216:TYR:CE2	2.48	0.48
1:A:190:GLN:OE1	2:A:2324:NDP:H2N	2.13	0.47
1:B:150:ALA:HA	1:B:153:LYS:HD3	1.96	0.47
1:B:53:HIS:HE1	1:B:128:LEU:HD11	1.77	0.47
1:B:17:PRO:HB2	1:B:48:HIS:HB2	1.96	0.47
1:B:250:ARG:HH11	1:B:282:GLN:NE2	2.08	0.47
1:A:81:TYR:O	1:A:111:VAL:HG13	2.15	0.46
1:B:10:LEU:C	1:B:12:ASP:N	2.69	0.46
1:B:133:GLU:HG3	1:B:133:GLU:H	1.35	0.46
1:B:9:LYS:NZ	1:B:13:GLY:HA2	2.30	0.45
1:A:96:ARG:HB3	1:A:97:PRO:HD3	1.99	0.45
1:A:219:LEU:HB2	2:A:2324:NDP:C5B	2.44	0.45
1:B:216:TYR:CZ	2:B:3324:NDP:H41N	2.51	0.45
1:A:103:LEU:CD1	1:A:111:VAL:HG23	2.47	0.44
1:A:153:LYS:HG2	1:A:154:CYS:N	2.32	0.44
1:B:273:ASN:CB	1:B:276:ARG:HD3	2.47	0.44
2:A:2324:NDP:H6N	2:A:2324:NDP:H3D	1.99	0.44
1:A:225:LYS:HD3	1:A:225:LYS:HA	1.78	0.44
1:B:193:CYS:HB3	1:B:215:ALA:CB	2.48	0.44
1:A:55:TYR:N	1:A:55:TYR:CD2	2.83	0.44
1:B:219:LEU:HD11	1:B:257:LEU:HD21	2.00	0.44
1:B:113:LEU:HD21	1:B:115:LEU:HD21	2.00	0.43
1:A:217:SER:H	2:A:2324:NDP:C5D	2.30	0.43
1:B:123:LYS:CD	1:B:124:PRO:HD2	2.35	0.43
1:B:60:GLN:NE2	1:B:60:GLN:N	2.65	0.43
1:A:5:GLN:HE22	1:A:19:LEU:HB3	1.84	0.43
1:B:187:VAL:O	1:B:212:VAL:HG13	2.19	0.42
1:B:96:ARG:HB3	1:B:97:PRO:HD3	2.01	0.42
1:A:258:ARG:NH2	1:A:287:GLN:HG3	2.34	0.42
1:B:43:GLU:OE1	1:B:68:LYS:HE2	2.20	0.42
1:B:22:GLY:HA3	2:B:3324:NDP:H4D	2.02	0.42
1:B:55:TYR:CD2	1:B:55:TYR:N	2.87	0.42
1:A:291:GLU:OE2	1:A:294:LYS:HE2	2.19	0.42
1:A:270:LYS:HD3	1:A:270:LYS:C	2.40	0.42
1:A:20:GLY:HA2	1:A:48:HIS:HB3	2.01	0.41
1:A:63:LEU:CD2	1:A:66:ARG:HH12	2.33	0.41
1:A:248:HIS:O	1:A:249:LYS:HB2	2.20	0.41
1:A:82:THR:HB	1:A:113:LEU:HB3	2.02	0.41
1:B:91:ARG:HG3	4:B:1064:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:HD3	1:B:225:LYS:HA	1.78	0.41
1:A:25:ALA:HB2	1:A:272:TYR:CZ	2.56	0.41
1:A:193:CYS:HB3	1:A:215:ALA:CB	2.50	0.41
1:A:91:ARG:HA	1:A:92:PRO:HD2	1.80	0.41
1:B:206:CYS:HB3	1:B:211:ILE:O	2.21	0.41
2:A:2324:NDP:H51N	2:A:2324:NDP:C6N	2.51	0.40
1:A:270:LYS:O	2:A:2324:NDP:H8A	2.21	0.40
1:A:31:ARG:O	1:A:60:GLN:HG2	2.21	0.40
1:A:316:ASN:HD22	1:A:316:ASN:HA	1.73	0.40
1:A:145:CYS:HB3	1:A:179:LYS:HD2	2.03	0.40
1:B:190:GLN:OE1	2:B:3324:NDP:H2N	2.22	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	317/323 (98%)	308 (97%)	9 (3%)	0	100	100
1	B	317/323 (98%)	306 (96%)	11 (4%)	0	100	100
All	All	634/646 (98%)	614 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	283/287 (99%)	260 (92%)	23 (8%)	15 3
1	B	283/287 (99%)	254 (90%)	29 (10%)	9 2
All	All	566/574 (99%)	514 (91%)	52 (9%)	11 2

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	31	ARG
1	A	59	GLU
1	A	75	LYS
1	A	82	THR
1	A	103	LEU
1	A	105	LYS
1	A	107	GLN
1	A	122	LEU
1	A	126	GLU
1	A	128	LEU
1	A	136	LYS
1	A	153	LYS
1	A	203	LEU
1	A	221	SER
1	A	225	LYS
1	A	246	LYS
1	A	249	LYS
1	A	254	LEU
1	A	261	LEU
1	A	268	LEU
1	A	299	LEU
1	A	304	HIS
1	B	6	GLN
1	B	12	ASP
1	B	19	LEU
1	B	31	ARG
1	B	33	LYS
1	B	60	GLN
1	B	68	LYS
1	B	82	THR
1	B	107	GLN
1	B	126	GLU
1	B	127	GLU
1	B	128	LEU

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Mol	Chain	Res	Type
1	B	133	GLU
1	B	136	LYS
1	B	170	ARG
1	B	171	ARG
1	B	183	LYS
1	B	199	ARG
1	B	203	LEU
1	B	212	VAL
1	B	223	ARG
1	B	225	LYS
1	B	246	LYS
1	B	249	LYS
1	B	254	LEU
1	B	258	ARG
1	B	268	LEU
1	B	287	GLN
1	B	299	LEU

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	53	HIS
1	A	56	ASN
1	A	60	GLN
1	A	134	ASN
1	A	178	ASN
1	A	262	GLN
1	A	282	GLN
1	A	302	ASN
1	A	316	ASN
1	B	5	GLN
1	B	53	HIS
1	B	56	ASN
1	B	60	GLN
1	B	101	ASN
1	B	178	ASN
1	B	262	GLN
1	B	282	GLN
1	B	287	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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	A	2324	-	42,52,52	1.69	8 (19%)	55,80,80	1.92	12 (21%)
3	RUT	A	2325	-	43,47,47	2.83	20 (46%)	60,71,71	2.32	13 (21%)
2	NDP	B	3324	-	42,52,52	1.66	7 (16%)	55,80,80	1.85	11 (20%)
3	RUT	B	3325	-	43,47,47	2.92	19 (44%)	60,71,71	2.27	13 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	2324	-	-	0/30/77/77	0/5/5/5
3	RUT	A	2325	-	-	0/13/53/53	0/5/5/5
2	NDP	B	3324	-	-	0/30/77/77	0/5/5/5
3	RUT	B	3325	-	-	0/13/53/53	0/5/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2324	NDP	C4N-C5N	-3.21	1.42	1.49
2	B	3324	NDP	C4N-C5N	-2.68	1.43	1.49
2	A	2324	NDP	PA-O1A	-2.51	1.42	1.51
2	B	3324	NDP	PA-O1A	-2.40	1.42	1.51
2	B	3324	NDP	O4D-C1D	2.15	1.47	1.42
2	A	2324	NDP	C4A-N3A	2.17	1.38	1.35
3	A	2325	RUT	O1-C8	2.22	1.40	1.37
3	A	2325	RUT	O16-C26	2.24	1.50	1.44
3	B	3325	RUT	O12-C21	2.39	1.48	1.43
2	A	2324	NDP	C3D-C4D	2.42	1.59	1.53
3	B	3325	RUT	O1-C8	2.47	1.41	1.37
2	B	3324	NDP	C6N-N1N	2.49	1.44	1.37
3	B	3325	RUT	C25-C24	2.49	1.58	1.52
3	A	2325	RUT	C25-C24	2.50	1.58	1.52
3	A	2325	RUT	O16-C22	2.53	1.48	1.41
3	A	2325	RUT	O12-C21	2.53	1.48	1.43
3	A	2325	RUT	O12-C22	2.62	1.44	1.40
3	A	2325	RUT	C9-C8	2.64	1.44	1.41
3	A	2325	RUT	C15-C14	2.71	1.43	1.38
3	B	3325	RUT	O16-C22	2.73	1.48	1.41
2	A	2324	NDP	C6N-N1N	2.91	1.46	1.37
3	B	3325	RUT	C9-C8	2.93	1.45	1.41
3	B	3325	RUT	O12-C22	2.93	1.45	1.40
3	B	3325	RUT	C15-C14	3.07	1.44	1.38
3	B	3325	RUT	C27-C26	3.28	1.59	1.51
3	A	2325	RUT	C27-C26	3.36	1.59	1.51
2	B	3324	NDP	C2A-N1A	3.53	1.40	1.33
3	B	3325	RUT	C19-C20	3.53	1.60	1.53
3	A	2325	RUT	C7-C6	3.61	1.44	1.37
3	A	2325	RUT	C19-C20	3.62	1.60	1.53
2	A	2324	NDP	C2A-N1A	3.65	1.40	1.33
3	B	3325	RUT	C25-C26	3.69	1.60	1.52
2	A	2324	NDP	C2A-N3A	3.75	1.38	1.32
3	B	3325	RUT	C7-C6	3.78	1.44	1.37
3	A	2325	RUT	C4-C9	3.82	1.50	1.43
3	A	2325	RUT	C18-C17	3.90	1.62	1.52
3	B	3325	RUT	C18-C17	3.94	1.62	1.52
2	B	3324	NDP	C2A-N3A	3.95	1.39	1.32
3	A	2325	RUT	C25-C26	4.04	1.61	1.52
3	B	3325	RUT	C4-C9	4.06	1.51	1.43
3	A	2325	RUT	O2-C16	4.33	1.48	1.41
2	A	2324	NDP	C6N-C5N	4.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3324	NDP	C6N-C5N	4.79	1.42	1.33
3	B	3325	RUT	O2-C16	4.93	1.49	1.41
3	A	2325	RUT	C10-C1	5.28	1.53	1.46
3	B	3325	RUT	C7-C8	5.51	1.48	1.37
3	A	2325	RUT	C7-C8	5.55	1.48	1.37
3	A	2325	RUT	C5-C6	5.68	1.48	1.39
3	B	3325	RUT	C5-C6	5.82	1.48	1.39
3	A	2325	RUT	C15-C10	5.94	1.52	1.39
3	B	3325	RUT	C15-C10	6.06	1.52	1.39
3	B	3325	RUT	C3-C9	6.09	1.49	1.41
3	B	3325	RUT	C10-C1	6.22	1.54	1.46
3	A	2325	RUT	C3-C9	6.31	1.50	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2325	RUT	C6-C7-C8	-12.24	109.12	120.42
3	B	3325	RUT	C6-C7-C8	-12.24	109.13	120.42
2	B	3324	NDP	N3A-C2A-N1A	-7.78	122.94	128.89
2	A	2324	NDP	N3A-C2A-N1A	-7.71	122.99	128.89
3	A	2325	RUT	C14-C15-C10	-5.60	112.97	121.14
3	B	3325	RUT	C14-C15-C10	-5.54	113.05	121.14
2	A	2324	NDP	O3-PA-O5B	-4.74	90.37	102.94
3	A	2325	RUT	O1-C1-C10	-4.32	106.99	113.14
2	B	3324	NDP	O3-PA-O5B	-4.22	91.73	102.94
2	A	2324	NDP	C1B-N9A-C4A	-3.76	121.26	126.94
3	B	3325	RUT	O1-C1-C10	-3.73	107.83	113.14
2	B	3324	NDP	C1B-N9A-C4A	-3.39	121.82	126.94
3	A	2325	RUT	O1-C8-C9	-3.10	117.95	121.15
3	B	3325	RUT	O1-C8-C9	-3.08	117.97	121.15
2	A	2324	NDP	C3N-C2N-N1N	-3.05	118.77	123.14
3	A	2325	RUT	O4-C4-C9	-3.04	114.89	121.37
3	A	2325	RUT	C4-C9-C8	-2.98	114.08	117.84
2	A	2324	NDP	O5B-C5B-C4B	-2.97	98.16	109.12
2	B	3324	NDP	C3N-C2N-N1N	-2.90	118.99	123.14
3	B	3325	RUT	O4-C4-C9	-2.89	115.20	121.37
3	B	3325	RUT	C4-C9-C8	-2.80	114.30	117.84
2	B	3324	NDP	O5B-C5B-C4B	-2.79	98.84	109.12
2	A	2324	NDP	O3-PN-O5D	-2.76	95.62	102.94
2	A	2324	NDP	O4B-C4B-C5B	-2.74	99.53	109.32
3	A	2325	RUT	O1-C8-C7	-2.71	112.72	116.18
3	A	2325	RUT	O5-C6-C7	-2.67	112.92	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2325	RUT	C27-C26-C25	-2.62	107.92	113.08
3	B	3325	RUT	O5-C6-C7	-2.62	113.08	121.04
2	B	3324	NDP	O4B-C4B-C5B	-2.61	99.98	109.32
3	B	3325	RUT	C27-C26-C25	-2.61	107.95	113.08
3	B	3325	RUT	O1-C8-C7	-2.55	112.93	116.18
2	A	2324	NDP	O4D-C4D-C5D	-2.51	100.34	109.32
3	B	3325	RUT	C4-C5-C6	-2.33	117.44	119.67
3	A	2325	RUT	C4-C5-C6	-2.30	117.47	119.67
3	A	2325	RUT	C24-C25-C26	-2.24	105.94	109.72
3	B	3325	RUT	C24-C25-C26	-2.10	106.18	109.72
2	A	2324	NDP	C5N-C4N-C3N	2.02	118.09	112.52
2	B	3324	NDP	C3B-C2B-C1B	2.04	106.67	102.73
2	B	3324	NDP	C5N-C4N-C3N	2.13	118.39	112.52
3	B	3325	RUT	C15-C10-C11	2.36	121.30	118.17
2	A	2324	NDP	O3X-P2B-O2X	2.36	116.38	107.38
2	B	3324	NDP	O3X-P2B-O2X	2.46	116.74	107.38
2	A	2324	NDP	O2A-PA-O1A	2.50	126.06	112.53
3	A	2325	RUT	C15-C10-C11	2.59	121.61	118.17
2	B	3324	NDP	O2A-PA-O1A	2.60	126.60	112.53
3	A	2325	RUT	C15-C14-C13	2.96	123.53	120.49
3	B	3325	RUT	C15-C14-C13	2.99	123.56	120.49
2	A	2324	NDP	C4B-O4B-C1B	3.91	114.02	109.72
2	B	3324	NDP	C4B-O4B-C1B	4.09	114.21	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2324	NDP	12	0
3	A	2325	RUT	1	0
2	B	3324	NDP	6	0
3	B	3325	RUT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	319/323 (98%)	-0.35	2 (0%)	90	92	6, 14, 32, 47	0
1	B	319/323 (98%)	-0.35	2 (0%)	90	92	7, 15, 34, 56	0
All	All	638/646 (98%)	-0.35	4 (0%)	90	92	6, 15, 33, 56	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	TRP	2.3
1	A	5	GLN	2.1
1	B	227	TRP	2.1
1	B	5	GLN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
2	NDP	A	2324	48/48	0.94	0.10	3.50	6,10,14,17	0
3	RUT	A	2325	43/43	0.84	0.12	1.24	12,29,37,40	0
3	RUT	B	3325	43/43	0.88	0.11	0.88	11,28,33,35	0
2	NDP	B	3324	48/48	0.96	0.08	0.49	6,11,16,18	0

6.5 Other polymers (i)

There are no such residues in this entry.