Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JKX
Title	:	Unexpected formation of an epoxide-derived multisubstrate adduct inhibitor on the active site of GAR transformylase
Authors	:	Greasley, S.E.; Marsilje, T.H.; Cai, H.; Baker, S.; Benkovic, S.J.; Boger, D.L.; Wilson, I.A.
Deposited on	:	2001-07-13
Resolution	:	1.60 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
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:

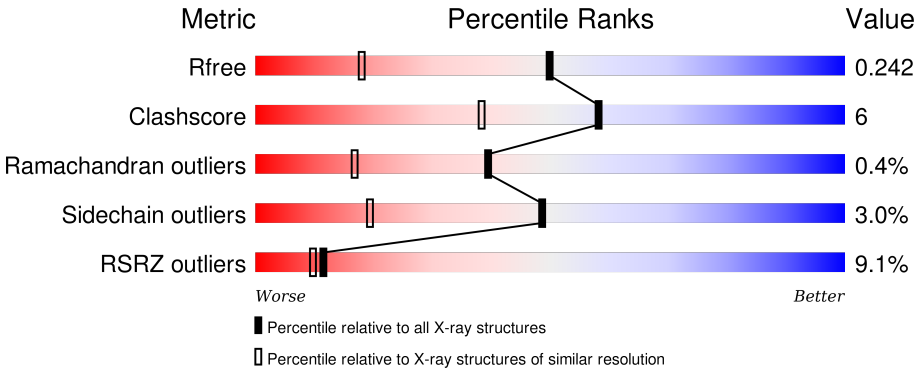
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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 >=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	212	2% 90% 8%
1	B	212	5% 88% 9%
1	C	212	7% 84% 13%
1	D	212	22% 77% 19%

2 Entry composition

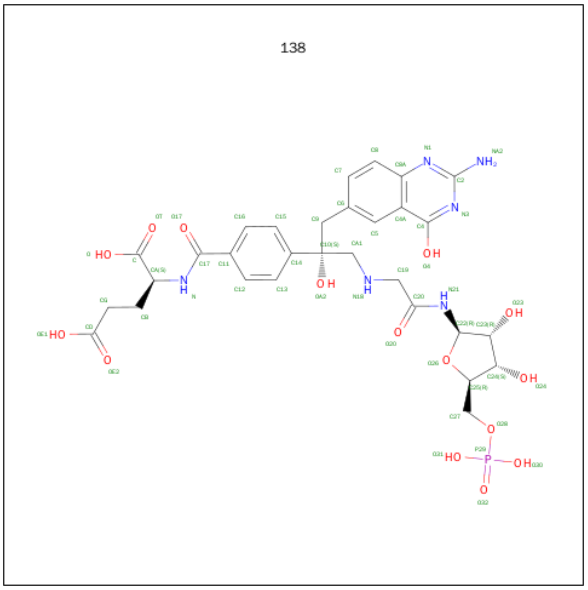
There are 3 unique types of molecules in this entry. The entry contains 7283 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	B	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	C	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	D	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			

- Molecule 2 is N-[5'-O-PHOSPHONO-RIBOFURANOSYL]-2-[2-HYDROXY-2-[4-[GLUTAMIC ACID]-N-CARBONYLPHENYL]-3-[2-AMINO-4-HYDROXY-QUINAZOLIN-6-YL]-PROPANYLAMINO]-ACETAMIDE (three-letter code: 138) (formula: $C_{30}H_{37}N_6O_{15}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	30	6	15	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			52	30	6	15	1		
2	C	1	Total	C	N	O	P	0	0
			52	30	6	15	1		
2	D	1	Total	C	N	O	P	0	0
			52	30	6	15	1		

- Molecule 3 is water.

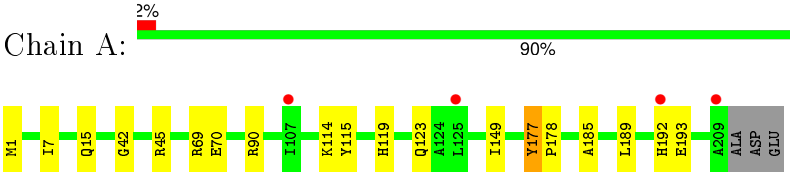
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		
3	B	181	Total	O	0	0
			181	181		
3	C	146	Total	O	0	0
			146	146		
3	D	108	Total	O	0	0
			108	108		

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.

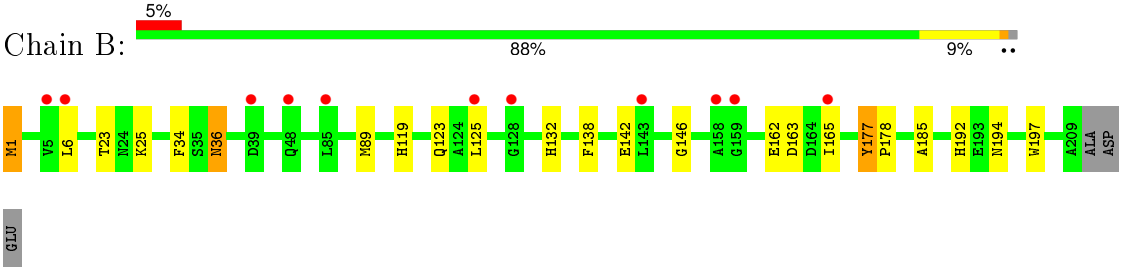
- Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain A:



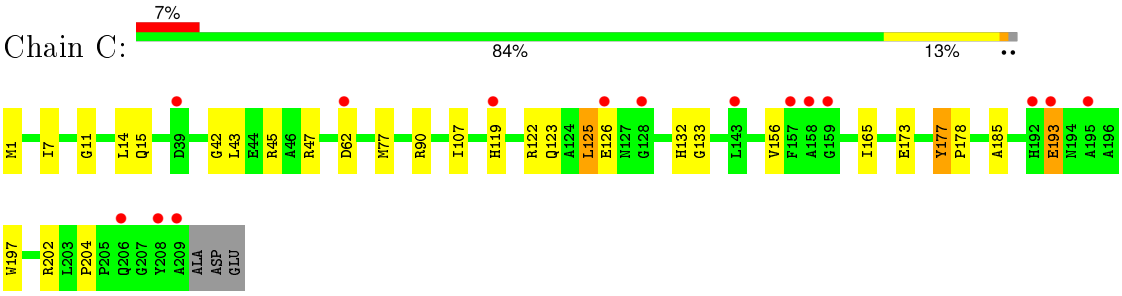
- Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain B:



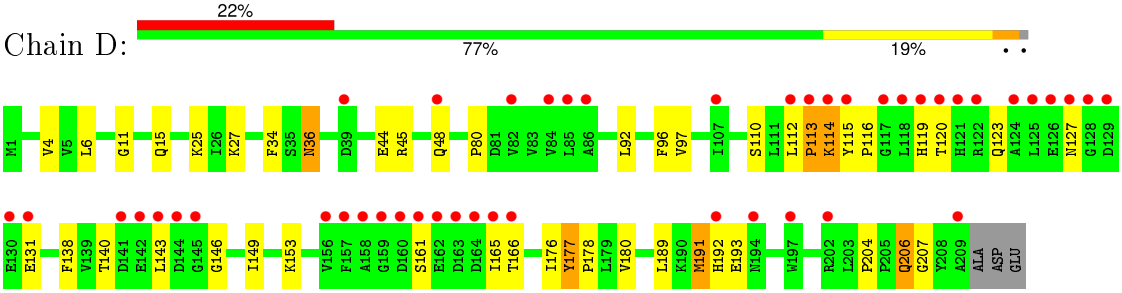
- Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain C:



- Molecule 1: PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.14Å 56.01Å 76.13Å 80.83° 71.71° 83.69°	Depositor
Resolution (Å)	30.00 – 1.60 27.59 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-1.60) 90.9 (27.59-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.243 0.221 , 0.242	Depositor DCC
R_{free} test set	10690 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 106828 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7283	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: 138

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	0.31	0/1654	0.58	0/2248
1	B	0.32	0/1654	0.58	0/2248
1	C	0.28	0/1654	0.56	0/2248
1	D	0.28	0/1654	0.54	0/2248
All	All	0.30	0/6616	0.56	0/8992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1617	0	1592	14	0
1	B	1617	0	1592	21	0
1	C	1617	0	1592	16	0
1	D	1617	0	1592	31	0
2	A	52	0	34	1	0
2	B	52	0	34	1	0
2	C	52	0	34	1	0
2	D	52	0	34	1	0
3	A	172	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	181	0	0	2	0
3	C	146	0	0	3	0
3	D	108	0	0	2	0
All	All	7283	0	6504	78	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 6.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ASN:HD22	1:D:36:ASN:H	1.27	0.80
1:B:36:ASN:H	1:B:36:ASN:HD22	1.30	0.79
1:D:44:GLU:O	1:D:48:GLN:HG2	1.82	0.79
1:D:206:GLN:NE2	1:D:206:GLN:H	1.81	0.78
1:C:122:ARG:O	1:C:126:GLU:HG2	1.92	0.69
1:D:119:HIS:O	1:D:123:GLN:HG3	1.93	0.68
1:D:115:TYR:N	1:D:116:PRO:HD3	2.12	0.65
1:C:77:MET:HE3	3:C:3255:HOH:O	1.97	0.64
1:D:206:GLN:HE21	1:D:206:GLN:H	1.43	0.63
1:D:161:SER:O	1:D:165:ILE:HG22	2.00	0.62
1:B:125:LEU:HD21	1:B:165:ILE:HG13	1.82	0.62
1:D:206:GLN:N	1:D:206:GLN:HE21	1.98	0.61
1:B:125:LEU:HD11	1:B:162:GLU:HA	1.83	0.60
1:D:15:GLN:HE21	1:D:45:ARG:HH11	1.50	0.60
1:B:6:LEU:HD22	1:B:34:PHE:HB2	1.83	0.59
1:A:1:MET:H1	1:B:1:MET:H1	1.49	0.59
1:C:156:VAL:HG22	1:C:165:ILE:HD11	1.87	0.56
1:B:192:HIS:HD2	3:B:2239:HOH:O	1.88	0.56
1:C:15:GLN:HE21	1:C:45:ARG:HH11	1.54	0.56
1:A:1:MET:N	1:B:1:MET:N	2.53	0.55
1:C:107:ILE:HD11	1:C:173:GLU:HG2	1.89	0.55
1:D:165:ILE:HG23	1:D:166:THR:N	2.23	0.54
1:D:6:LEU:HD22	1:D:34:PHE:HB2	1.90	0.54
1:A:149:ILE:HD13	1:A:189:LEU:HD21	1.89	0.53
1:B:142:GLU:OE2	1:B:194:ASN:HB3	2.09	0.52
1:B:192:HIS:HE1	3:B:2277:HOH:O	1.92	0.52
1:D:165:ILE:HG23	1:D:166:THR:H	1.77	0.50
1:A:1:MET:H1	1:B:1:MET:N	2.08	0.50
1:D:177:TYR:HB3	1:D:178:PRO:HD3	1.94	0.49
1:C:177:TYR:HB3	1:C:178:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:O	1:C:123:GLN:HG3	2.13	0.48
1:D:192:HIS:O	1:D:193:GLU:HB2	2.14	0.48
1:D:110:SER:HB3	1:D:120:THR:HB	1.95	0.48
1:D:27:LYS:HE3	3:D:4284:HOH:O	2.14	0.47
1:C:197:TRP:CE2	1:C:202:ARG:HG3	2.49	0.47
1:C:1:MET:HE2	1:C:185:ALA:HB2	1.97	0.47
1:D:11:GLY:HA2	3:D:4224:HOH:O	2.15	0.47
1:B:119:HIS:O	1:B:123:GLN:HG3	2.15	0.47
1:D:113:PRO:O	1:D:114:LYS:C	2.53	0.47
1:A:1:MET:HE1	1:A:185:ALA:HA	1.97	0.46
1:D:176:ILE:O	1:D:180:VAL:HG23	2.15	0.46
1:A:15:GLN:HE21	1:A:45:ARG:HH11	1.63	0.46
1:B:89:MET:HA	2:B:2221:138:H15	1.97	0.46
1:D:115:TYR:CD2	1:D:115:TYR:N	2.79	0.46
1:B:1:MET:HE2	1:B:185:ALA:HB2	1.97	0.46
1:D:140:THR:HG21	1:D:191:MET:CE	2.46	0.46
1:D:131:GLU:OE2	1:D:153:LYS:HD3	2.16	0.45
1:A:1:MET:H2	1:B:1:MET:H2	1.64	0.45
1:B:138:PHE:O	1:B:146:GLY:HA3	2.17	0.45
1:C:125:LEU:HA	1:C:125:LEU:HD12	1.90	0.44
1:D:36:ASN:ND2	1:D:36:ASN:H	2.07	0.44
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.99	0.43
1:A:90:ARG:O	2:A:1221:138:H8	2.18	0.43
1:D:138:PHE:O	1:D:146:GLY:HA3	2.19	0.43
1:D:97:VAL:HG21	2:D:4221:138:NA2	2.34	0.43
1:D:112:LEU:HA	1:D:113:PRO:C	2.39	0.43
1:C:11:GLY:HA2	3:C:3224:HOH:O	2.17	0.43
1:B:192:HIS:HB2	1:B:197:TRP:NE1	2.33	0.43
1:A:1:MET:HE2	1:A:185:ALA:HB2	2.01	0.43
1:A:119:HIS:O	1:A:123:GLN:HG3	2.18	0.43
1:D:4:VAL:HG23	1:D:80:PRO:HB3	2.02	0.42
1:C:43:LEU:O	1:C:47:ARG:HG3	2.19	0.42
1:A:114:LYS:HG2	1:A:115:TYR:CD2	2.55	0.42
1:B:132:HIS:HD2	1:B:165:ILE:HG22	1.84	0.42
1:D:92:LEU:HD13	1:D:96:PHE:CE1	2.54	0.42
1:B:36:ASN:HD22	1:B:36:ASN:N	2.05	0.42
1:C:204:PRO:HB2	3:C:3299:HOH:O	2.19	0.42
1:A:7:ILE:CD1	1:A:42:GLY:HA3	2.50	0.41
1:A:177:TYR:HB3	1:A:178:PRO:HD3	2.01	0.41
1:D:149:ILE:HD13	1:D:189:LEU:HD21	2.02	0.41
1:D:113:PRO:O	1:D:114:LYS:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:CD1	1:C:42:GLY:HA3	2.49	0.41
1:C:90:ARG:O	2:C:3221:138:H8	2.21	0.41
1:C:132:HIS:CG	1:C:133:GLY:H	2.39	0.41
1:D:204:PRO:HG2	1:D:207:GLY:O	2.21	0.40
1:B:36:ASN:ND2	1:B:36:ASN:H	2.09	0.40
1:A:69:ARG:NH2	3:A:1339:HOH:O	2.54	0.40
1:B:23:THR:OG1	1:B:25:LYS:HG3	2.21	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	207/212 (98%)	206 (100%)	1 (0%)	0	100 100
1	B	207/212 (98%)	203 (98%)	4 (2%)	0	100 100
1	C	207/212 (98%)	202 (98%)	4 (2%)	1 (0%)	34 12
1	D	207/212 (98%)	199 (96%)	6 (3%)	2 (1%)	19 4
All	All	828/848 (98%)	810 (98%)	15 (2%)	3 (0%)	39 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	193	GLU
1	D	113	PRO
1	D	114	LYS

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	169/171 (99%)	165 (98%)	4 (2%)	57 27
1	B	169/171 (99%)	165 (98%)	4 (2%)	57 27
1	C	169/171 (99%)	164 (97%)	5 (3%)	48 19
1	D	169/171 (99%)	162 (96%)	7 (4%)	37 11
All	All	676/684 (99%)	656 (97%)	20 (3%)	48 19

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLU
1	A	177	TYR
1	A	192	HIS
1	A	193	GLU
1	B	1	MET
1	B	36	ASN
1	B	163	ASP
1	B	177	TYR
1	C	14	LEU
1	C	62	ASP
1	C	125	LEU
1	C	177	TYR
1	C	193	GLU
1	D	25	LYS
1	D	36	ASN
1	D	127	ASN
1	D	143	LEU
1	D	177	TYR
1	D	191	MET
1	D	206	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	99	HIS
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	36	ASN
1	B	192	HIS
1	B	201	GLN
1	C	15	GLN
1	D	15	GLN
1	D	36	ASN
1	D	192	HIS
1	D	206	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	138	A	1221	-	49,55,55	3.10	23 (46%)	56,80,80	1.63	9 (16%)
2	138	B	2221	-	49,55,55	3.03	21 (42%)	56,80,80	1.67	9 (16%)
2	138	C	3221	-	49,55,55	3.14	23 (46%)	56,80,80	1.70	10 (17%)
2	138	D	4221	-	49,55,55	3.28	24 (48%)	56,80,80	1.67	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	138	A	1221	-	-	0/39/61/61	0/4/4/4
2	138	B	2221	-	-	0/39/61/61	0/4/4/4
2	138	C	3221	-	-	0/39/61/61	0/4/4/4
2	138	D	4221	-	-	0/39/61/61	0/4/4/4

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3221	138	P29-O32	-2.76	1.42	1.51
2	B	2221	138	P29-O32	-2.69	1.42	1.51
2	D	4221	138	P29-O32	-2.63	1.42	1.51
2	A	1221	138	P29-O32	-2.41	1.43	1.51
2	A	1221	138	C15-C16	2.07	1.42	1.38
2	A	1221	138	C4A-C8A	2.15	1.45	1.42
2	C	3221	138	C4-N3	2.15	1.42	1.36
2	B	2221	138	C16-C11	2.21	1.43	1.39
2	B	2221	138	CA1-C10	2.25	1.56	1.53
2	B	2221	138	C4A-C8A	2.27	1.46	1.42
2	A	1221	138	C4-N3	2.29	1.42	1.36
2	D	4221	138	C4-N3	2.34	1.42	1.36
2	D	4221	138	CA1-C10	2.35	1.56	1.53
2	A	1221	138	C12-C13	2.39	1.43	1.38
2	C	3221	138	C16-C11	2.39	1.43	1.39
2	C	3221	138	C4A-C8A	2.44	1.46	1.42
2	C	3221	138	CA1-C10	2.44	1.56	1.53
2	C	3221	138	C22-N21	2.45	1.46	1.43
2	A	1221	138	CA1-C10	2.46	1.56	1.53
2	D	4221	138	C15-C16	2.49	1.43	1.38
2	A	1221	138	C16-C11	2.53	1.43	1.39
2	D	4221	138	C4A-C8A	2.58	1.46	1.42
2	D	4221	138	C16-C11	2.60	1.43	1.39
2	B	2221	138	C8A-N1	2.62	1.42	1.37
2	B	2221	138	C9-C6	2.62	1.56	1.51
2	B	2221	138	C12-C13	2.69	1.43	1.38
2	A	1221	138	C5-C6	2.72	1.44	1.37
2	D	4221	138	C22-N21	2.73	1.46	1.43
2	A	1221	138	C9-C6	2.75	1.56	1.51
2	C	3221	138	C12-C13	2.80	1.43	1.38
2	B	2221	138	O4-C4	2.82	1.41	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1221	138	O4-C4	2.86	1.41	1.28
2	D	4221	138	C12-C13	2.88	1.43	1.38
2	A	1221	138	CB-CA	2.97	1.57	1.53
2	C	3221	138	C8A-N1	2.99	1.42	1.37
2	C	3221	138	C5-C6	2.99	1.44	1.37
2	B	2221	138	C5-C6	3.00	1.44	1.37
2	C	3221	138	O4-C4	3.07	1.42	1.28
2	D	4221	138	C8A-N1	3.08	1.42	1.37
2	A	1221	138	C8A-N1	3.12	1.43	1.37
2	D	4221	138	O4-C4	3.20	1.43	1.28
2	D	4221	138	C5-C6	3.24	1.45	1.37
2	C	3221	138	C9-C6	3.25	1.57	1.51
2	C	3221	138	CB-CA	3.26	1.57	1.53
2	A	1221	138	C12-C11	3.27	1.44	1.39
2	B	2221	138	C8-C7	3.33	1.43	1.36
2	B	2221	138	C7-C6	3.46	1.46	1.38
2	A	1221	138	C8-C7	3.52	1.44	1.36
2	A	1221	138	C7-C6	3.57	1.46	1.38
2	D	4221	138	C9-C6	3.58	1.57	1.51
2	B	2221	138	C12-C11	3.63	1.45	1.39
2	B	2221	138	CB-CA	3.64	1.58	1.53
2	C	3221	138	C12-C11	3.66	1.45	1.39
2	C	3221	138	C8-C7	3.68	1.44	1.36
2	D	4221	138	C8-C7	3.69	1.44	1.36
2	C	3221	138	C7-C6	3.70	1.46	1.38
2	B	2221	138	C2-N3	3.75	1.42	1.35
2	C	3221	138	C2-N3	3.78	1.42	1.35
2	D	4221	138	C7-C6	3.78	1.46	1.38
2	D	4221	138	CB-CA	3.79	1.58	1.53
2	D	4221	138	C12-C11	3.80	1.45	1.39
2	A	1221	138	C2-N3	3.87	1.42	1.35
2	D	4221	138	C2-N3	4.12	1.42	1.35
2	A	1221	138	C13-C14	4.35	1.46	1.39
2	B	2221	138	C15-C14	4.58	1.46	1.39
2	B	2221	138	C13-C14	4.60	1.46	1.39
2	C	3221	138	C13-C14	4.64	1.46	1.39
2	D	4221	138	C13-C14	4.72	1.46	1.39
2	A	1221	138	C15-C14	4.76	1.46	1.39
2	C	3221	138	C15-C14	4.87	1.46	1.39
2	D	4221	138	C15-C14	5.00	1.47	1.39
2	B	2221	138	C10-C14	5.67	1.58	1.53
2	C	3221	138	C9-C10	5.88	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2221	138	C2-NA2	5.93	1.46	1.34
2	B	2221	138	CA1-N18	5.98	1.54	1.46
2	D	4221	138	C9-C10	6.05	1.63	1.54
2	C	3221	138	C2-NA2	6.18	1.46	1.34
2	A	1221	138	C9-C10	6.23	1.64	1.54
2	D	4221	138	C2-NA2	6.23	1.46	1.34
2	A	1221	138	C2-NA2	6.24	1.46	1.34
2	A	1221	138	CA1-N18	6.35	1.54	1.46
2	B	2221	138	C9-C10	6.39	1.64	1.54
2	C	3221	138	C10-C14	6.50	1.59	1.53
2	C	3221	138	CA1-N18	6.56	1.55	1.46
2	A	1221	138	C10-C14	6.81	1.59	1.53
2	D	4221	138	CA1-N18	6.94	1.55	1.46
2	D	4221	138	C10-C14	7.19	1.59	1.53
2	C	3221	138	O17-C17	10.31	1.44	1.23
2	B	2221	138	O17-C17	10.42	1.44	1.23
2	A	1221	138	O17-C17	10.44	1.44	1.23
2	D	4221	138	O17-C17	10.45	1.44	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3221	138	O17-C17-C11	-6.18	110.40	120.97
2	D	4221	138	O17-C17-C11	-5.95	110.80	120.97
2	B	2221	138	O17-C17-C11	-5.94	110.81	120.97
2	A	1221	138	O17-C17-C11	-5.76	111.12	120.97
2	D	4221	138	N1-C2-N3	-4.95	119.91	127.44
2	B	2221	138	N1-C2-N3	-4.95	119.91	127.44
2	C	3221	138	N1-C2-N3	-4.91	119.96	127.44
2	A	1221	138	N1-C2-N3	-4.87	120.03	127.44
2	A	1221	138	C4A-C8A-N1	-3.45	119.53	122.90
2	C	3221	138	C4A-C8A-N1	-3.35	119.63	122.90
2	B	2221	138	C4A-C8A-N1	-3.22	119.76	122.90
2	D	4221	138	C4A-C8A-N1	-3.20	119.77	122.90
2	B	2221	138	CA1-C10-C14	-2.69	103.77	110.75
2	C	3221	138	CA1-C10-C14	-2.56	104.11	110.75
2	A	1221	138	O30-P29-O28	-2.48	99.43	106.56
2	D	4221	138	O30-P29-O28	-2.45	99.50	106.56
2	C	3221	138	O30-P29-O28	-2.38	99.71	106.56
2	A	1221	138	CA1-C10-C14	-2.34	104.68	110.75
2	B	2221	138	O30-P29-O28	-2.20	100.22	106.56
2	D	4221	138	CA1-C10-C14	-2.20	105.03	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3221	138	C19-N18-CA1	-2.04	106.97	115.27
2	B	2221	138	O28-P29-O32	2.06	112.38	107.14
2	A	1221	138	CG-CB-CA	2.06	117.17	112.99
2	C	3221	138	O28-P29-O32	2.18	112.68	107.14
2	A	1221	138	O28-P29-O32	2.21	112.77	107.14
2	C	3221	138	O4-C4-C4A	2.23	121.48	116.59
2	D	4221	138	O4-C4-C4A	2.26	121.53	116.59
2	A	1221	138	O4-C4-C4A	2.27	121.56	116.59
2	D	4221	138	O28-P29-O32	2.29	112.96	107.14
2	B	2221	138	O4-C4-C4A	2.33	121.70	116.59
2	C	3221	138	CG-CB-CA	3.05	119.18	112.99
2	B	2221	138	CG-CB-CA	3.29	119.67	112.99
2	D	4221	138	CG-CB-CA	3.33	119.76	112.99
2	A	1221	138	C11-C17-N	3.55	123.25	116.93
2	D	4221	138	C11-C17-N	3.56	123.26	116.93
2	B	2221	138	C11-C17-N	3.72	123.55	116.93
2	C	3221	138	C11-C17-N	3.72	123.56	116.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1221	138	1	0
2	B	2221	138	1	0
2	C	3221	138	1	0
2	D	4221	138	1	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^{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	209/212 (98%)	0.13	4 (1%) 70 68	9, 17, 29, 39	0
1	B	209/212 (98%)	0.25	11 (5%) 30 27	10, 17, 33, 39	0
1	C	209/212 (98%)	0.48	15 (7%) 18 16	16, 24, 38, 48	0
1	D	209/212 (98%)	1.03	46 (22%) 1 1	15, 26, 46, 54	0
All	All	836/848 (98%)	0.47	76 (9%) 11 10	9, 21, 41, 54	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	143	LEU	8.5
1	D	118	LEU	5.8
1	D	159	GLY	5.8
1	D	125	LEU	5.3
1	D	161	SER	4.9
1	C	193	GLU	4.9
1	B	158	ALA	4.8
1	D	141	ASP	4.6
1	B	159	GLY	4.6
1	D	113	PRO	4.6
1	D	115	TYR	4.5
1	D	158	ALA	4.4
1	C	159	GLY	4.3
1	D	163	ASP	4.1
1	B	125	LEU	4.0
1	C	143	LEU	4.0
1	D	39	ASP	3.9
1	D	122	ARG	3.9
1	D	142	GLU	3.8
1	C	209	ALA	3.8
1	D	126	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	114	LYS	3.6
1	D	120	THR	3.6
1	D	165	ILE	3.5
1	D	128	GLY	3.4
1	D	127	ASN	3.4
1	C	192	HIS	3.3
1	D	121	HIS	3.3
1	B	39	ASP	3.3
1	D	164	ASP	3.2
1	A	209	ALA	3.2
1	A	192	HIS	3.2
1	D	197	TRP	3.1
1	D	112	LEU	3.0
1	D	131	GLU	3.0
1	D	119	HIS	3.0
1	D	209	ALA	3.0
1	C	126	GLU	3.0
1	A	125	LEU	3.0
1	C	157	PHE	3.0
1	D	162	GLU	3.0
1	D	84	VAL	2.9
1	D	85	LEU	2.9
1	D	156	VAL	2.8
1	D	130	GLU	2.8
1	C	158	ALA	2.7
1	D	166	THR	2.7
1	B	143	LEU	2.7
1	D	202	ARG	2.7
1	B	85	LEU	2.6
1	D	194	ASN	2.5
1	C	62	ASP	2.5
1	D	124	ALA	2.5
1	C	119	HIS	2.4
1	D	48	GLN	2.4
1	B	6	LEU	2.3
1	D	192	HIS	2.3
1	C	195	ALA	2.2
1	D	129	ASP	2.2
1	A	107	ILE	2.2
1	D	144	ASP	2.2
1	D	145	GLY	2.2
1	B	128	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	86	ALA	2.2
1	D	160	ASP	2.2
1	B	165	ILE	2.2
1	C	206	GLN	2.2
1	C	128	GLY	2.1
1	D	117	GLY	2.1
1	C	39	ASP	2.1
1	B	5	VAL	2.1
1	D	107	ILE	2.1
1	D	82	VAL	2.0
1	C	208	TYR	2.0
1	B	48	GLN	2.0
1	D	157	PHE	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	138	C	3221	52/52	0.89	0.13	0.63	19,24,39,44	0
2	138	A	1221	52/52	0.94	0.13	0.62	10,16,39,44	0
2	138	D	4221	52/52	0.86	0.16	0.38	26,31,43,46	0
2	138	B	2221	52/52	0.93	0.12	0.05	14,18,40,44	0

6.5 Other polymers

There are no such residues in this entry.