Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:33 AM GMT

PDB ID	:	2XIQ
Title	:	Crystal structure of human methylmalonyl-CoA mutase in complex with adenosylcobalamin and malonyl-CoA
Authors	:	Yue, W.W.; Froese, D.S.; Kochan, G.; Chaikuad, A.; Krojer, T.; Muniz, J.; Ugochukwu, E.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Bountra, C.; Oppermann, U.
Deposited on	:	2010-06-30
Resolution	:	1.95 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:

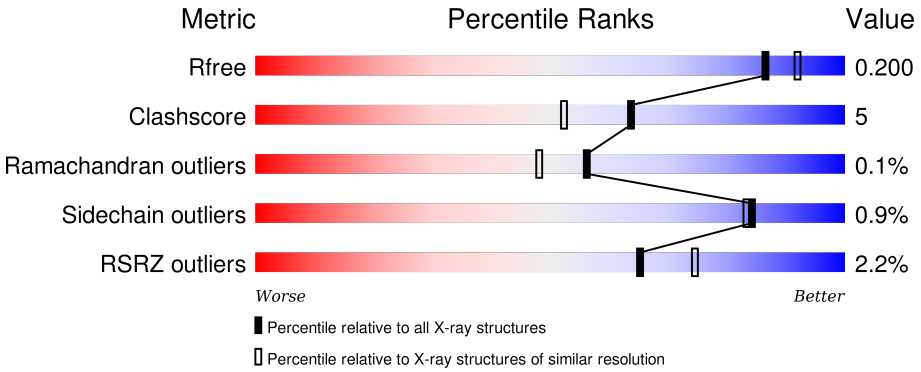
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	762	2% 86% 7% 6%
1	B	762	2% 87% 6% 6%

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	B12	A	3001	X	-	X	-
2	B12	B	3001	X	-	-	-
3	5AD	A	4001[A]	-	-	-	X
3	5AD	A	4001[B]	-	-	X	X
3	5AD	B	4001[A]	-	-	-	X
3	5AD	B	4001[B]	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12511 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 METHYLMALONYL-COA MUTASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	3	0
			5531	3497	957	1045	32			
1	B	713	Total	C	N	O	S	0	2	0
			5512	3486	953	1041	32			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP P22033
A	751	ALA	-	EXPRESSION TAG	UNP P22033
A	752	GLU	-	EXPRESSION TAG	UNP P22033
A	753	ASN	-	EXPRESSION TAG	UNP P22033
A	754	LEU	-	EXPRESSION TAG	UNP P22033
A	755	TYR	-	EXPRESSION TAG	UNP P22033
A	756	PHE	-	EXPRESSION TAG	UNP P22033
A	757	GLN	-	EXPRESSION TAG	UNP P22033
A	758	SER	-	EXPRESSION TAG	UNP P22033
A	759	HIS	-	EXPRESSION TAG	UNP P22033
A	760	HIS	-	EXPRESSION TAG	UNP P22033
A	761	HIS	-	EXPRESSION TAG	UNP P22033
A	762	HIS	-	EXPRESSION TAG	UNP P22033
A	763	HIS	-	EXPRESSION TAG	UNP P22033
A	764	HIS	-	EXPRESSION TAG	UNP P22033
A	765	ASP	-	EXPRESSION TAG	UNP P22033
A	766	TYR	-	EXPRESSION TAG	UNP P22033
A	767	LYS	-	EXPRESSION TAG	UNP P22033
A	768	ASP	-	EXPRESSION TAG	UNP P22033
A	769	ASP	-	EXPRESSION TAG	UNP P22033
A	770	ASP	-	EXPRESSION TAG	UNP P22033
A	771	ASP	-	EXPRESSION TAG	UNP P22033
A	772	LYS	-	EXPRESSION TAG	UNP P22033
A	499	THR	ALA	CONFLICT	UNP P22033
B	11	MET	-	EXPRESSION TAG	UNP P22033

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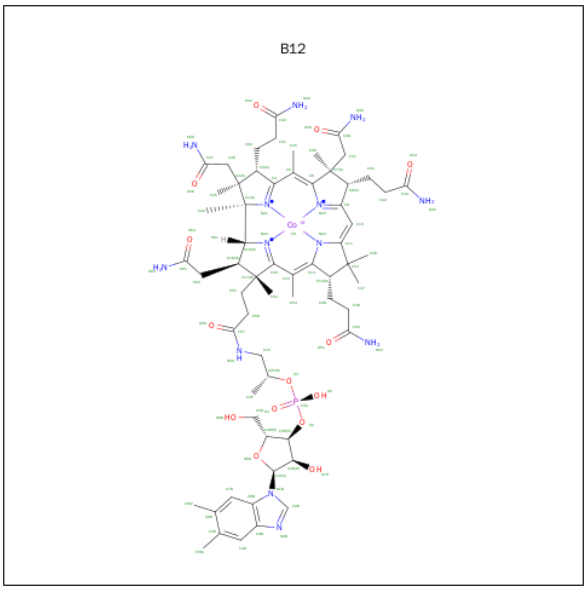
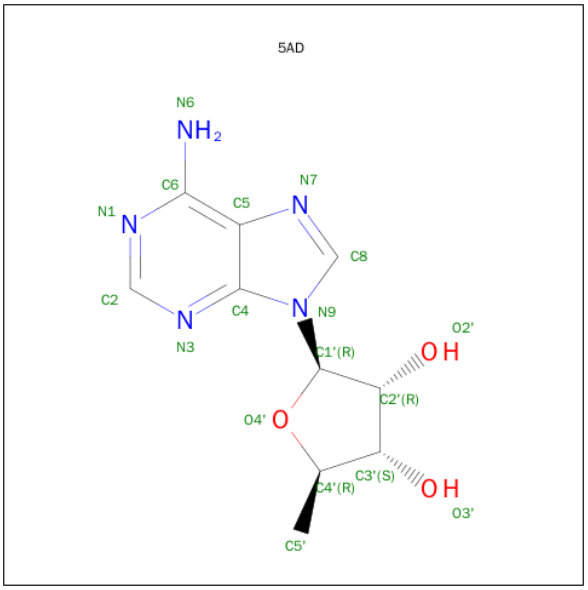
Chain	Residue	Modelled	Actual	Comment	Reference
B	751	ALA	-	EXPRESSION TAG	UNP P22033
B	752	GLU	-	EXPRESSION TAG	UNP P22033
B	753	ASN	-	EXPRESSION TAG	UNP P22033
B	754	LEU	-	EXPRESSION TAG	UNP P22033
B	755	TYR	-	EXPRESSION TAG	UNP P22033
B	756	PHE	-	EXPRESSION TAG	UNP P22033
B	757	GLN	-	EXPRESSION TAG	UNP P22033
B	758	SER	-	EXPRESSION TAG	UNP P22033
B	759	HIS	-	EXPRESSION TAG	UNP P22033
B	760	HIS	-	EXPRESSION TAG	UNP P22033
B	761	HIS	-	EXPRESSION TAG	UNP P22033
B	762	HIS	-	EXPRESSION TAG	UNP P22033
B	763	HIS	-	EXPRESSION TAG	UNP P22033
B	764	HIS	-	EXPRESSION TAG	UNP P22033
B	765	ASP	-	EXPRESSION TAG	UNP P22033
B	766	TYR	-	EXPRESSION TAG	UNP P22033
B	767	LYS	-	EXPRESSION TAG	UNP P22033
B	768	ASP	-	EXPRESSION TAG	UNP P22033
B	769	ASP	-	EXPRESSION TAG	UNP P22033
B	770	ASP	-	EXPRESSION TAG	UNP P22033
B	771	ASP	-	EXPRESSION TAG	UNP P22033
B	772	LYS	-	EXPRESSION TAG	UNP P22033
B	499	THR	ALA	CONFLICT	UNP P22033

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



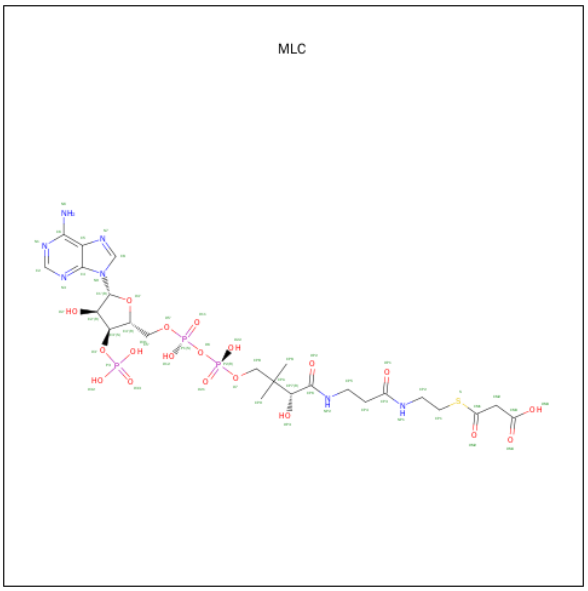
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			36	20	10	6		
3	B	1	Total	C	N	O	0	1
			36	20	10	6		

- Molecule 4 is MALONYL-COENZYME A (three-letter code: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		

- Molecule 5 is water.

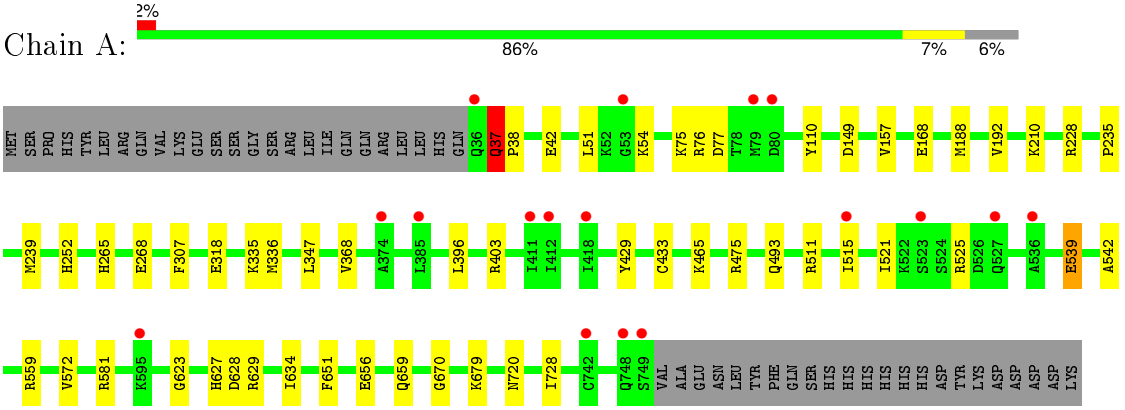
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	494	Total	O	0	0
			494	494		
5	B	612	Total	O	0	0
			612	612		

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.

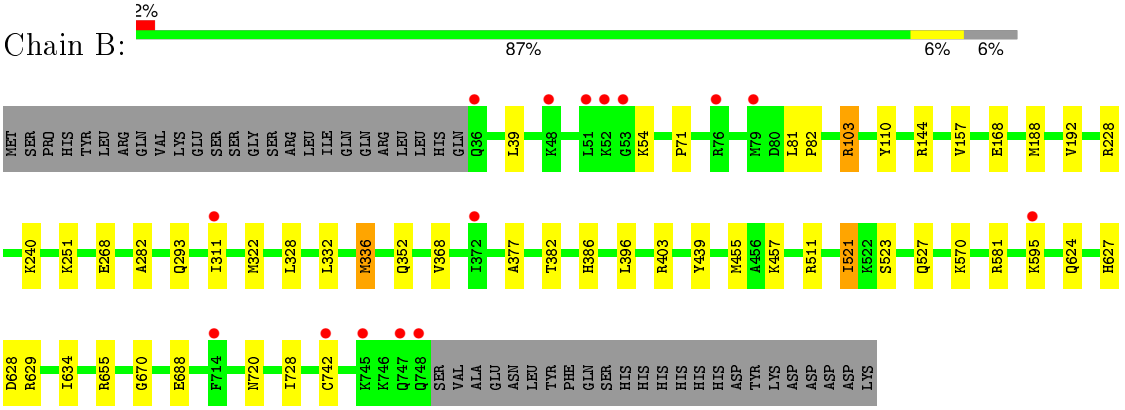
- Molecule 1: METHYLMALONYL-COA MUTASE, MITOCHONDRIAL

Chain A:



- Molecule 1: METHYLMALONYL-COA MUTASE, MITOCHONDRIAL

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.65Å 143.62Å 163.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.82 – 1.95 52.08 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (107.82-1.95) 99.2 (52.08-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0066	Depositor
R, R_{free}	0.161 , 0.201 0.161 , 0.200	Depositor DCC
R_{free} test set	6447 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.9	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 128908 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12511	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: MLC, B12, 5AD

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	0.68	2/5646 (0.0%)	0.51	0/7634
1	B	0.71	0/5624	0.54	0/7606
All	All	0.70	2/11270 (0.0%)	0.52	0/15240

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	GLU	CD-OE2	10.63	1.37	1.25
1	A	539	GLU	CD-OE1	-6.50	1.18	1.25

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	5531	0	5521	46	0
1	B	5512	0	5497	39	0
2	A	91	0	87	21	0
2	B	91	0	87	18	0
3	A	36	0	26	11	0
3	B	36	0	26	12	0
4	A	54	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	54	0	34	4	0
5	A	494	0	0	17	1
5	B	612	0	0	11	1
All	All	12511	0	11311	117	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (117) 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)
2:B:3001:B12:H531	2:B:3001:B12:H552	1.34	1.09
2:A:3001:B12:H552	2:A:3001:B12:H531	1.45	0.97
1:A:465:LYS:NZ	5:A:2296:HOH:O	1.94	0.95
1:A:656:GLU:HG3	5:A:2428:HOH:O	1.71	0.90
2:A:3001:B12:H372	3:A:4001[B]:5AD:H2	1.52	0.89
2:B:3001:B12:H372	3:B:4001[B]:5AD:H2	1.55	0.87
1:B:368:VAL:HG23	5:B:2298:HOH:O	1.76	0.84
2:B:3001:B12:H531	2:B:3001:B12:C55	2.10	0.82
3:B:4001[B]:5AD:H8	5:B:2308:HOH:O	1.80	0.80
1:B:403[B]:ARG:HD3	5:B:2324:HOH:O	1.79	0.80
1:B:634:ILE:HD13	1:B:728:ILE:HD13	1.64	0.80
2:B:3001:B12:H261	3:B:4001[B]:5AD:H3'	1.63	0.79
1:A:368:VAL:HG23	5:A:2226:HOH:O	1.86	0.75
3:A:4001[B]:5AD:H8	5:A:2493:HOH:O	1.86	0.75
2:A:3001:B12:H261	3:A:4001[B]:5AD:H3'	1.68	0.75
1:A:42:GLU:HB2	5:A:2004:HOH:O	1.86	0.74
3:A:4001[B]:5AD:O4'	3:A:4001[B]:5AD:N3	2.20	0.73
3:B:4001[B]:5AD:N3	3:B:4001[B]:5AD:O4'	2.16	0.73
2:A:3001:B12:C55	2:A:3001:B12:H531	2.17	0.73
1:A:37:GLN:H	1:A:38:PRO:HD2	1.53	0.72
1:A:525:ARG:HD2	5:A:2359:HOH:O	1.89	0.72
1:A:525:ARG:HB2	5:A:2359:HOH:O	1.89	0.71
1:A:168:GLU:HG3	1:A:521:ILE:HD11	1.73	0.70
1:A:403[A]:ARG:HD3	5:A:2251:HOH:O	1.90	0.69
2:B:3001:B12:H351	2:B:3001:B12:H362	1.75	0.69
1:B:168:GLU:HG3	1:B:521:ILE:HD11	1.74	0.67
1:A:37:GLN:H	1:A:38:PRO:CD	2.07	0.67
1:A:629:ARG:H	2:A:3001:B12:H522	1.41	0.66
1:A:581:ARG:HD2	5:A:2371:HOH:O	1.94	0.66
1:B:629:ARG:H	2:B:3001:B12:H522	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HG3	5:A:2323:HOH:O	1.96	0.65
1:B:628:ASP:H	2:B:3001:B12:H522	1.45	0.64
1:B:240:LYS:NZ	5:B:2211:HOH:O	2.31	0.63
1:B:527:GLN:HB2	5:B:2441:HOH:O	1.99	0.62
1:B:570:LYS:NZ	5:B:2485:HOH:O	2.33	0.61
1:B:54:LYS:HB3	5:B:2005:HOH:O	2.00	0.61
2:A:3001:B12:H362	2:A:3001:B12:H351	1.82	0.61
1:B:332:LEU:O	1:B:336:MET:HG2	2.00	0.60
1:B:634:ILE:HD13	1:B:728:ILE:CD1	2.32	0.59
1:B:627:HIS:NE2	2:B:3001:B12:N21	2.49	0.59
2:A:3001:B12:H372	2:A:3001:B12:H351	1.85	0.58
1:B:168:GLU:CG	1:B:521:ILE:HD11	2.34	0.57
1:B:742:CYS:HB2	5:B:2596:HOH:O	2.06	0.56
1:B:396:LEU:HD22	3:B:4001[A]:5AD:N6	2.22	0.55
2:B:3001:B12:N22	3:B:4001[B]:5AD:H5'2	2.21	0.55
1:B:457:LYS:NZ	5:B:2370:HOH:O	2.40	0.55
1:A:627:HIS:NE2	2:A:3001:B12:N21	2.54	0.55
1:A:559:ARG:HB2	5:A:2359:HOH:O	2.07	0.54
1:A:628:ASP:H	2:A:3001:B12:H522	1.54	0.53
2:B:3001:B12:H291	3:B:4001[A]:5AD:C8	2.22	0.53
1:B:332:LEU:O	1:B:336:MET:CG	2.56	0.53
2:A:3001:B12:N29	3:A:4001[B]:5AD:H2'	2.23	0.53
1:A:228:ARG:NH2	2:A:3001:B12:H401	2.07	0.52
1:A:670:GLY:HA3	2:A:3001:B12:HM53	1.92	0.52
1:B:268:GLU:HB3	2:B:3001:B12:H532	1.92	0.51
1:A:268:GLU:HB3	2:A:3001:B12:H532	1.91	0.51
1:A:396:LEU:HD22	3:A:4001[A]:5AD:N6	2.26	0.51
1:A:403[B]:ARG:NH1	5:A:2250:HOH:O	2.44	0.49
3:B:4001[A]:5AD:H5'1	4:B:5001:MLC:HM22	1.95	0.49
1:A:37:GLN:N	1:A:38:PRO:HD2	2.24	0.49
1:A:335:LYS:HG2	1:A:336:MET:CE	2.43	0.49
2:A:3001:B12:N22	3:A:4001[B]:5AD:C5'	2.75	0.48
1:B:157:VAL:HG11	1:B:511:ARG:HA	1.96	0.48
2:B:3001:B12:C35	2:B:3001:B12:H362	2.43	0.48
2:A:3001:B12:N22	3:A:4001[B]:5AD:H5'2	2.28	0.48
1:A:307:PHE:CD1	1:A:347:LEU:HG	2.48	0.48
5:A:2423:HOH:O	1:B:581:ARG:HD2	2.14	0.48
1:B:251:LYS:HD3	1:B:251:LYS:HA	1.74	0.47
1:B:655:ARG:HD3	1:B:688:GLU:OE1	2.15	0.47
1:B:103:ARG:HD3	4:B:5001:MLC:C8	2.45	0.46
1:B:110:TYR:CE2	4:B:5001:MLC:HM21	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3001:B12:H362	2:A:3001:B12:C35	2.46	0.46
1:A:188:MET:HG3	1:A:192:VAL:HA	1.98	0.46
1:A:623:GLY:O	1:A:651:PHE:HA	2.15	0.46
1:A:51:LEU:HB3	1:A:54:LYS:HB2	1.98	0.46
1:B:188:MET:HG3	1:B:192:VAL:HA	1.97	0.46
2:A:3001:B12:N22	3:A:4001[A]:5AD:H5'2	2.32	0.45
1:A:634:ILE:HD13	1:A:728:ILE:HG12	1.99	0.45
2:B:3001:B12:N22	3:B:4001[A]:5AD:H5'2	2.32	0.45
2:B:3001:B12:N22	3:B:4001[B]:5AD:C5'	2.79	0.45
1:B:144:ARG:HD3	1:B:624:GLN:OE1	2.17	0.45
1:B:670:GLY:HA3	2:B:3001:B12:HM53	1.98	0.45
1:B:228:ARG:NH2	2:B:3001:B12:H401	2.15	0.45
1:A:542:ALA:HA	1:A:572:VAL:HG11	1.99	0.45
1:A:149:ASP:HB3	1:A:515:ILE:HG12	1.98	0.44
2:A:3001:B12:C5	3:A:4001[A]:5AD:H8	2.47	0.44
1:B:311:ILE:HG13	1:B:377:ALA:HB2	2.00	0.44
1:A:110:TYR:CE2	4:A:5001:MLC:HM21	2.53	0.44
1:B:352:GLN:HG3	1:B:386:HIS:CD2	2.53	0.44
3:A:4001[A]:5AD:H5'1	4:A:5001:MLC:HM22	2.00	0.44
1:A:210:LYS:HD2	1:A:252:HIS:HB3	2.00	0.43
1:A:210:LYS:HG2	5:A:2126:HOH:O	2.18	0.43
1:B:328:LEU:HG	1:B:439:TYR:CD2	2.54	0.43
1:A:539:GLU:OE1	1:A:539:GLU:HA	2.19	0.43
1:A:157:VAL:HG11	1:A:511:ARG:HA	2.01	0.43
1:B:627:HIS:CD2	2:B:3001:B12:N23	2.86	0.43
2:B:3001:B12:C53	2:B:3001:B12:C55	2.90	0.43
1:A:659:GLN:NE2	5:B:2370:HOH:O	2.52	0.43
1:A:77:ASP:HB3	1:A:433:CYS:SG	2.59	0.43
1:B:322:MET:HE1	1:B:382:THR:HB	2.00	0.43
1:A:656:GLU:CG	5:A:2428:HOH:O	2.47	0.42
1:A:525:ARG:CB	5:A:2359:HOH:O	2.61	0.42
1:A:235:PRO:O	1:A:239:MET:HG2	2.20	0.42
1:B:352:GLN:HE22	3:B:4001[B]:5AD:H4'	1.85	0.41
1:A:37:GLN:HE21	1:A:37:GLN:HB2	1.75	0.41
1:B:39:LEU:HD21	1:B:71:PRO:HD2	2.02	0.41
1:A:228:ARG:HD2	1:A:265:HIS:CD2	2.55	0.41
1:B:282:ALA:HB1	1:B:455:MET:HG2	2.02	0.41
1:A:75:LYS:HA	1:A:429:TYR:CE1	2.56	0.41
1:A:318:GLU:OE1	1:A:318:GLU:HA	2.21	0.41
1:B:81:LEU:HA	1:B:82:PRO:HD3	1.97	0.40
3:B:4001[A]:5AD:H5'1	4:B:5001:MLC:CM2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3001:B12:C53	2:A:3001:B12:C55	2.96	0.40
2:A:3001:B12:H301	2:A:3001:B12:H253	1.76	0.40
1:A:627:HIS:CE1	2:A:3001:B12:H421	2.57	0.40
1:A:679:LYS:HB2	5:A:2446:HOH:O	2.22	0.40
1:B:595:LYS:HG2	5:B:2220:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2219:HOH:O	5:B:2334:HOH:O[2_565]	2.17	0.03

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	715/762 (94%)	702 (98%)	12 (2%)	1 (0%)	56	48
1	B	713/762 (94%)	699 (98%)	14 (2%)	0	100	100
All	All	1428/1524 (94%)	1401 (98%)	26 (2%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

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	583/636 (92%)	579 (99%)	4 (1%)	88 88
1	B	580/636 (91%)	574 (99%)	6 (1%)	82 80
All	All	1163/1272 (91%)	1153 (99%)	10 (1%)	84 83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	76	ARG
1	A	475	ARG
1	A	720	ASN
1	B	103	ARG
1	B	293	GLN
1	B	336	MET
1	B	521	ILE
1	B	523	SER
1	B	720	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	314	ASN
1	A	605	HIS
1	B	293	GLN
1	B	314	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	B12	A	3001	1	74,101,101	1.17	5 (6%)	111,166,166	1.63	15 (13%
3	5AD	A	4001[A]	-	15,20,20	3.16	5 (33%)	14,30,30	5.78	4 (28%
3	5AD	A	4001[B]	-	15,20,20	2.90	5 (33%)	14,30,30	5.70	6 (42%
4	MLC	A	5001	-	42,56,56	2.18	10 (23%)	54,83,83	3.02	6 (11%
2	B12	B	3001	1	74,101,101	1.17	6 (8%)	111,166,166	1.60	11 (9%
3	5AD	B	4001[A]	-	15,20,20	3.11	5 (33%)	14,30,30	5.73	6 (42%
3	5AD	B	4001[B]	-	15,20,20	3.00	6 (40%)	14,30,30	5.68	6 (42%
4	MLC	B	5001	-	42,56,56	1.97	7 (16%)	54,83,83	2.80	6 (11%

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	B12	A	3001	1	1/1/36/38	0/51/223/223	0/3/11/11
3	5AD	A	4001[A]	-	-	0/0/20/20	0/3/3/3
3	5AD	A	4001[B]	-	-	0/0/20/20	0/3/3/3
4	MLC	A	5001	-	-	0/48/71/71	0/3/3/3
2	B12	B	3001	1	1/1/36/38	0/51/223/223	0/3/11/11
3	5AD	B	4001[A]	-	-	0/0/20/20	0/3/3/3
3	5AD	B	4001[B]	-	-	0/0/20/20	0/3/3/3
4	MLC	B	5001	-	-	0/48/71/71	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4001[A]	5AD	C3'-C4'	-9.50	1.41	1.53
3	B	4001[A]	5AD	C3'-C4'	-9.22	1.41	1.53
3	B	4001[B]	5AD	C3'-C4'	-8.97	1.41	1.53
3	A	4001[B]	5AD	C3'-C4'	-8.46	1.42	1.53
3	A	4001[A]	5AD	C3'-C2'	-5.07	1.39	1.53
3	B	4001[A]	5AD	C3'-C2'	-5.03	1.39	1.53
3	B	4001[B]	5AD	C3'-C2'	-4.90	1.40	1.53
3	A	4001[B]	5AD	C3'-C2'	-4.86	1.40	1.53
2	A	3001	B12	C8B-N1B	-3.96	1.33	1.38
2	A	3001	B12	C11-C10	-3.89	1.34	1.41
2	B	3001	B12	C8B-N1B	-3.70	1.33	1.38
2	B	3001	B12	C11-C10	-3.48	1.34	1.41
2	B	3001	B12	C2-C3	-3.45	1.52	1.58
4	A	5001	MLC	C2'-C3'	-3.07	1.46	1.53
3	A	4001[A]	5AD	C5'-C4'	-2.95	1.44	1.51
3	B	4001[A]	5AD	C5'-C4'	-2.91	1.44	1.51
3	B	4001[B]	5AD	C5'-C4'	-2.88	1.44	1.51
3	A	4001[B]	5AD	C5'-C4'	-2.69	1.45	1.51
4	A	5001	MLC	OP3-CP7	-2.68	1.36	1.42
2	A	3001	B12	C2-C3	-2.58	1.54	1.58
4	A	5001	MLC	CP8-CPA	-2.33	1.48	1.53
4	B	5001	MLC	CP8-CPA	-2.19	1.49	1.53
4	A	5001	MLC	O2'-C2'	-2.09	1.38	1.43
4	B	5001	MLC	C5'-C4'	-2.08	1.44	1.51
4	A	5001	MLC	C5'-C4'	-2.06	1.45	1.51
4	B	5001	MLC	O3'-C3'	-2.02	1.37	1.44
4	A	5001	MLC	O3'-C3'	-2.00	1.37	1.44
3	B	4001[B]	5AD	C4-N3	2.03	1.38	1.35
3	B	4001[B]	5AD	O4'-C4'	2.33	1.49	1.44
3	B	4001[B]	5AD	C6-N6	2.42	1.42	1.34
3	A	4001[B]	5AD	C6-N6	2.43	1.42	1.34
4	B	5001	MLC	C6-N6	2.44	1.42	1.34
2	B	3001	B12	O6R-C1R	2.62	1.44	1.41
3	A	4001[B]	5AD	O4'-C4'	2.67	1.50	1.44
3	A	4001[A]	5AD	C6-N6	2.73	1.43	1.34
2	B	3001	B12	C6B-C5B	2.74	1.48	1.41
3	B	4001[A]	5AD	C6-N6	2.79	1.43	1.34
3	A	4001[A]	5AD	O4'-C4'	2.79	1.50	1.44
4	A	5001	MLC	C6-N6	2.85	1.43	1.34
4	B	5001	MLC	CP3-NP1	2.90	1.40	1.33
3	B	4001[A]	5AD	O4'-C4'	2.99	1.51	1.44
2	B	3001	B12	C8B-C9B	3.00	1.46	1.40
4	B	5001	MLC	CP6-NP2	3.66	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	B12	C6B-C5B	3.72	1.51	1.41
2	A	3001	B12	C8B-C9B	4.03	1.48	1.40
4	A	5001	MLC	CP3-NP1	4.34	1.43	1.33
4	A	5001	MLC	CP6-NP2	4.72	1.43	1.33
4	B	5001	MLC	OM2-CM1	9.49	1.36	1.21
4	A	5001	MLC	OM2-CM1	9.65	1.36	1.21

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5001	MLC	OM2-CM1-S	-18.19	108.40	122.83
3	A	4001[A]	5AD	C1'-N9-C4	-17.33	100.80	126.94
3	B	4001[A]	5AD	C1'-N9-C4	-17.04	101.23	126.94
4	B	5001	MLC	OM2-CM1-S	-16.85	109.46	122.83
3	B	4001[B]	5AD	C1'-N9-C4	-15.84	103.05	126.94
3	A	4001[B]	5AD	C1'-N9-C4	-15.65	103.33	126.94
3	B	4001[A]	5AD	N3-C2-N1	-9.95	121.28	128.89
3	A	4001[A]	5AD	N3-C2-N1	-9.93	121.29	128.89
4	A	5001	MLC	N3-C2-N1	-9.67	121.49	128.89
3	B	4001[B]	5AD	N3-C2-N1	-9.04	121.97	128.89
3	A	4001[B]	5AD	N3-C2-N1	-8.80	122.16	128.89
3	B	4001[B]	5AD	C4'-O4'-C1'	-8.56	100.31	109.72
3	A	4001[B]	5AD	C4'-O4'-C1'	-8.52	100.35	109.72
4	B	5001	MLC	N3-C2-N1	-8.36	122.49	128.89
3	A	4001[A]	5AD	C5'-C4'-C3'	-7.03	108.45	115.80
3	B	4001[A]	5AD	C5'-C4'-C3'	-6.86	108.63	115.80
3	A	4001[B]	5AD	C5'-C4'-C3'	-5.65	109.90	115.80
3	B	4001[B]	5AD	C5'-C4'-C3'	-4.77	110.82	115.80
2	B	3001	B12	C9-C10-C11	-4.70	120.50	132.28
2	A	3001	B12	C9-C10-C11	-4.68	120.56	132.28
2	A	3001	B12	C20-C1-C19	-3.71	105.74	109.38
2	B	3001	B12	C3-C4-C5	-3.39	120.43	131.88
4	B	5001	MLC	C4-C5-N7	-3.28	106.46	109.48
4	B	5001	MLC	CM2-CM1-S	-3.27	110.23	113.50
2	B	3001	B12	C30-C3-C2	-3.24	112.70	119.11
2	A	3001	B12	C3-C4-C5	-3.21	121.04	131.88
3	A	4001[A]	5AD	C4'-O4'-C1'	-3.19	106.22	109.72
3	B	4001[A]	5AD	C4'-O4'-C1'	-3.04	106.38	109.72
2	A	3001	B12	C20-C1-N21	-2.99	99.54	108.29
2	B	3001	B12	C20-C1-N21	-2.96	99.62	108.29
4	A	5001	MLC	C4-C5-N7	-2.91	106.80	109.48
4	B	5001	MLC	P2-O6-P1	-2.85	124.74	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3001	B12	C30-C3-C2	-2.81	113.55	119.11
2	A	3001	B12	C2P-C1P-N59	-2.71	108.91	112.92
2	B	3001	B12	C13-C14-C15	-2.48	123.52	131.88
2	A	3001	B12	C13-C14-C15	-2.37	123.87	131.88
2	A	3001	B12	C25-C2-C3	-2.21	111.82	115.56
2	B	3001	B12	C25-C2-C3	-2.16	111.91	115.56
3	B	4001[A]	5AD	C4-C5-N7	-2.10	107.54	109.48
4	A	5001	MLC	CM2-CM1-S	-2.09	111.41	113.50
2	A	3001	B12	C53-C15-C14	-2.04	114.59	118.25
2	A	3001	B12	C55-C56-C57	-2.03	106.96	111.06
2	B	3001	B12	C2P-C1P-N59	-2.01	109.95	112.92
2	A	3001	B12	O2-P-O3	2.15	102.11	100.07
4	B	5001	MLC	CP8-CPA-CPB	2.18	111.33	108.50
4	A	5001	MLC	O6-P2-O7	2.22	108.84	102.94
3	B	4001[A]	5AD	C2'-C1'-N9	2.28	117.78	114.29
4	A	5001	MLC	O7-CPB-CPA	2.39	114.39	110.55
3	A	4001[B]	5AD	O4'-C1'-N9	2.76	113.87	108.10
3	B	4001[B]	5AD	O4'-C1'-N9	2.76	113.88	108.10
2	B	3001	B12	C53-C15-C16	3.09	123.79	118.25
2	A	3001	B12	C53-C15-C16	3.14	123.87	118.25
3	B	4001[B]	5AD	C2'-C1'-N9	3.30	119.33	114.29
2	A	3001	B12	C26-C2-C1	3.61	115.75	110.00
3	A	4001[B]	5AD	C2'-C1'-N9	3.95	120.33	114.29
2	B	3001	B12	C19-C1-N21	4.25	106.48	102.16
2	B	3001	B12	C26-C2-C1	4.34	116.91	110.00
2	A	3001	B12	C19-C1-N21	5.16	107.41	102.16
2	A	3001	B12	C1-C19-N24	9.98	118.30	106.20
2	B	3001	B12	C1-C19-N24	10.28	118.67	106.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3001	B12	C19
2	A	3001	B12	C19

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	B12	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4001[A]	5AD	4	0
3	A	4001[B]	5AD	7	0
4	A	5001	MLC	2	0
2	B	3001	B12	18	0
3	B	4001[A]	5AD	5	0
3	B	4001[B]	5AD	7	0
4	B	5001	MLC	4	0

5.7 Other polymers

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	714/762 (93%)	0.01	17 (2%)	62	72	19, 33, 62, 93	0
1	B	713/762 (93%)	-0.17	15 (2%)	67	75	14, 26, 51, 87	0
All	All	1427/1524 (93%)	-0.08	32 (2%)	65	74	14, 30, 57, 93	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	GLN	5.1
1	A	36	GLN	4.8
1	A	749	SER	4.1
1	B	742	CYS	3.6
1	B	51	LEU	3.4
1	A	748	GLN	3.1
1	B	79	MET	3.1
1	A	79	MET	2.9
1	B	714	PHE	2.9
1	B	53	GLY	2.8
1	A	53	GLY	2.6
1	B	372	ILE	2.5
1	B	52	LYS	2.5
1	A	527	GLN	2.4
1	B	76	ARG	2.4
1	A	412	ILE	2.3
1	B	748	GLN	2.3
1	A	80	ASP	2.3
1	B	745	LYS	2.3
1	A	742	CYS	2.2
1	A	418	ILE	2.2
1	A	515	ILE	2.2
1	A	536	ALA	2.2
1	B	48	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	2.2
1	B	311	ILE	2.2
1	B	595	LYS	2.2
1	A	374	ALA	2.1
1	A	385	LEU	2.1
1	A	523	SER	2.1
1	A	595	LYS	2.0
1	B	747	GLN	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^{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
3	5AD	B	4001[B]	18/18	0.64	0.40	10.92	33,75,120,137	18
3	5AD	B	4001[A]	18/18	0.64	0.40	10.77	38,58,74,78	18
3	5AD	A	4001[B]	18/18	0.57	0.45	9.10	36,58,87,88	18
3	5AD	A	4001[A]	18/18	0.57	0.45	8.95	56,106,143,145	18
2	B12	B	3001	91/91	0.97	0.12	1.05	12,19,24,33	0
2	B12	A	3001	91/91	0.97	0.12	0.88	15,22,31,35	0
4	MLC	B	5001	54/54	0.97	0.10	0.04	13,21,34,53	0
4	MLC	A	5001	54/54	0.95	0.11	-0.32	18,28,41,49	0

6.5 Other polymers (i)

There are no such residues in this entry.