Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:20 PM GMT

PDB ID	:	1T7L
Title	:	Crystal Structure of Cobalamin-Independent Methionine Synthase from T. maritima
Authors	:	Pejchal, R.; Ludwig, M.L.
Deposited on	:	2004-05-10
Resolution	:	2.00 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:

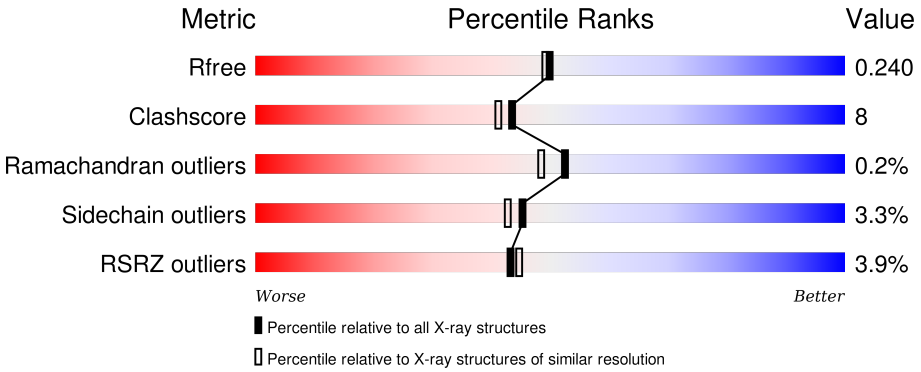
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	766	3% 78% 15%
1	B	766	4% 77% 17% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MRY	A	1353	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12255 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5831	3780	950	1077	24			
1	B	731	Total	C	N	O	S	0	0	0
			5780	3743	950	1063	24			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	EXPRESSION TAG	UNP Q9X112
A	-30	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-29	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-28	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-27	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-26	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-25	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-24	GLY	-	EXPRESSION TAG	UNP Q9X112
A	-23	LYS	-	EXPRESSION TAG	UNP Q9X112
A	-22	PRO	-	EXPRESSION TAG	UNP Q9X112
A	-21	ILE	-	EXPRESSION TAG	UNP Q9X112
A	-20	PRO	-	EXPRESSION TAG	UNP Q9X112
A	-19	ASN	-	EXPRESSION TAG	UNP Q9X112
A	-18	PRO	-	EXPRESSION TAG	UNP Q9X112
A	-17	LEU	-	EXPRESSION TAG	UNP Q9X112
A	-16	LEU	-	EXPRESSION TAG	UNP Q9X112
A	-15	GLY	-	EXPRESSION TAG	UNP Q9X112
A	-14	LEU	-	EXPRESSION TAG	UNP Q9X112
A	-13	ASP	-	EXPRESSION TAG	UNP Q9X112
A	-12	SER	-	EXPRESSION TAG	UNP Q9X112
A	-11	THR	-	EXPRESSION TAG	UNP Q9X112
A	-10	GLU	-	EXPRESSION TAG	UNP Q9X112
A	-9	ASN	-	EXPRESSION TAG	UNP Q9X112
A	-8	LEU	-	EXPRESSION TAG	UNP Q9X112

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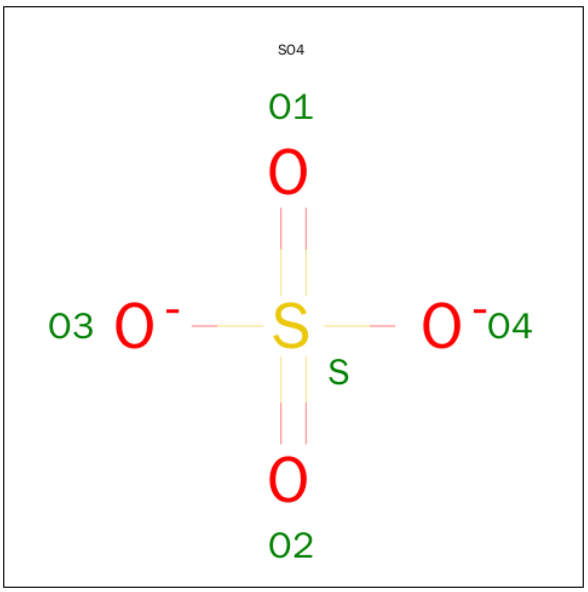
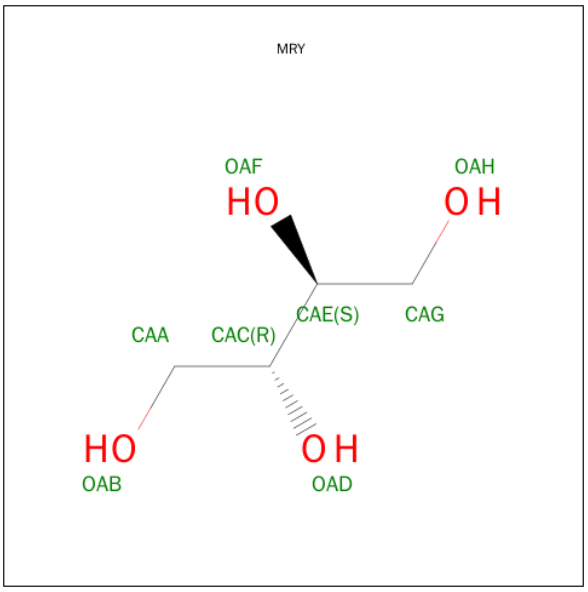
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	TYR	-	EXPRESSION TAG	UNP Q9X112
A	-6	PHE	-	EXPRESSION TAG	UNP Q9X112
A	-5	GLN	-	EXPRESSION TAG	UNP Q9X112
A	-4	GLN	-	EXPRESSION TAG	UNP Q9X112
A	-3	ILE	-	EXPRESSION TAG	UNP Q9X112
A	-2	ASP	-	EXPRESSION TAG	UNP Q9X112
A	-1	PRO	-	EXPRESSION TAG	UNP Q9X112
A	0	PHE	-	EXPRESSION TAG	UNP Q9X112
A	1	THR	-	EXPRESSION TAG	UNP Q9X112
B	-31	MET	-	EXPRESSION TAG	UNP Q9X112
B	-30	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-29	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-28	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-27	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-26	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-25	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-24	GLY	-	EXPRESSION TAG	UNP Q9X112
B	-23	LYS	-	EXPRESSION TAG	UNP Q9X112
B	-22	PRO	-	EXPRESSION TAG	UNP Q9X112
B	-21	ILE	-	EXPRESSION TAG	UNP Q9X112
B	-20	PRO	-	EXPRESSION TAG	UNP Q9X112
B	-19	ASN	-	EXPRESSION TAG	UNP Q9X112
B	-18	PRO	-	EXPRESSION TAG	UNP Q9X112
B	-17	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-16	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-15	GLY	-	EXPRESSION TAG	UNP Q9X112
B	-14	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-13	ASP	-	EXPRESSION TAG	UNP Q9X112
B	-12	SER	-	EXPRESSION TAG	UNP Q9X112
B	-11	THR	-	EXPRESSION TAG	UNP Q9X112
B	-10	GLU	-	EXPRESSION TAG	UNP Q9X112
B	-9	ASN	-	EXPRESSION TAG	UNP Q9X112
B	-8	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-7	TYR	-	EXPRESSION TAG	UNP Q9X112
B	-6	PHE	-	EXPRESSION TAG	UNP Q9X112
B	-5	GLN	-	EXPRESSION TAG	UNP Q9X112
B	-4	GLN	-	EXPRESSION TAG	UNP Q9X112
B	-3	ILE	-	EXPRESSION TAG	UNP Q9X112
B	-2	ASP	-	EXPRESSION TAG	UNP Q9X112
B	-1	PRO	-	EXPRESSION TAG	UNP Q9X112
B	0	PHE	-	EXPRESSION TAG	UNP Q9X112
B	1	THR	-	EXPRESSION TAG	UNP Q9X112

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 8 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0

- Molecule 4 is water.

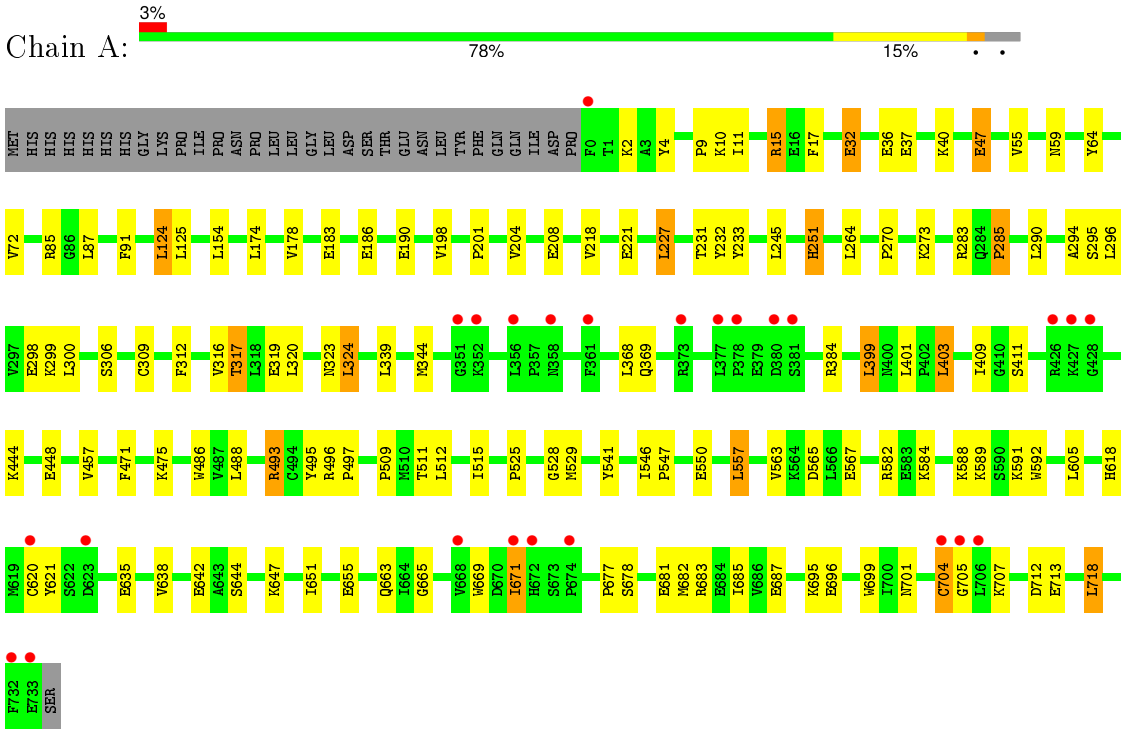
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	331	Total O 331 331	0	0
4	B	287	Total O 287 287	0	0

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.

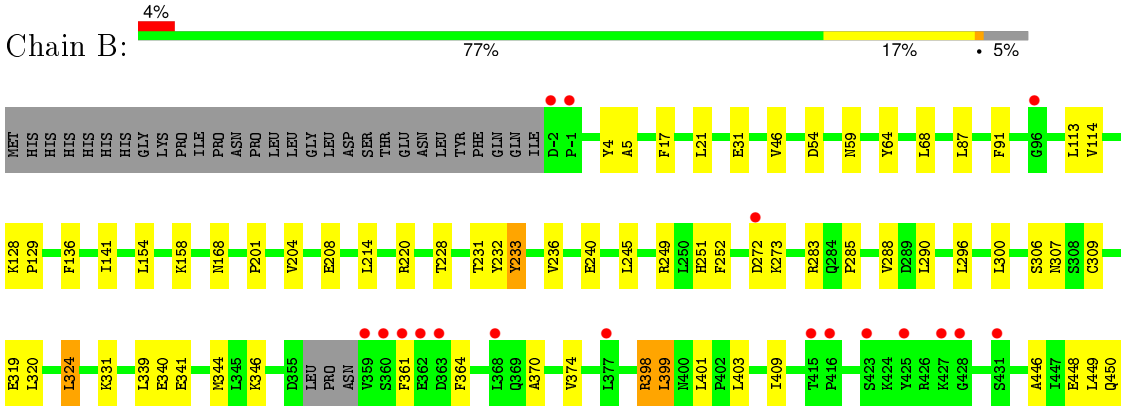
- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase

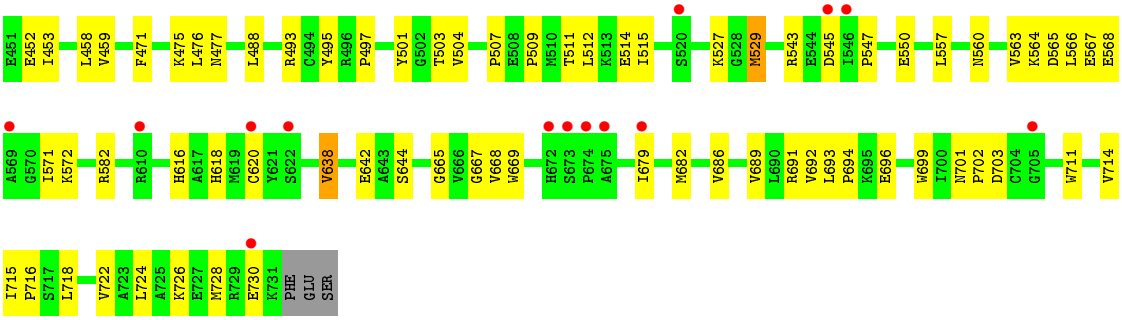
Chain A:



- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase

Chain B:




E451 E452 I453 L458 V459 F471 K475 L476 N477 L488 R493 C494 Y495 R496 P497 Y501 G502 T503 V504 P507 E508 P509 M510 T511 L512 K513 E514 I515 S520 K527 G528 M529 R543 E544 D545 I546 P547 E550 L557 N560 V563 K564 D565 L566 E567 E568
A569 G570 I571 K572 R582 R610 H616 A617 H618 M619 C620 Y621 S622 V638 E642 A643 S644 G665 V666 G667 V668 W669 H672 S673 P674 A675 I679 M682 V686 V689 L690 R691 V692 L693 P694 K695 E696 W699 I700 N701 P702 D703 C704 G705 W711 V714
I715 P716 S717 L718 V722 A723 L724 A725 K726 E727 M728 R729 E730 K731 PHE GLU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.56Å 158.76Å 64.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.00 19.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.91-2.00) 99.3 (19.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.240 0.206 , 0.240	Depositor DCC
R_{free} test set	11262 reflections (10.00%)	DCC
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.9	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 112572 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12255	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: MRY, SO4

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	0/5977	0.57	1/8117 (0.0%)
1	B	0.34	0/5924	0.56	0/8046
All	All	0.33	0/11901	0.57	1/16163 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	528	GLY	N-CA-C	-5.84	98.50	113.10

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	5831	0	5632	91	0
1	B	5780	0	5551	97	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	8	0	10	0	0
3	B	8	0	10	0	0
4	A	331	0	0	7	0
4	B	287	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12255	0	11203	185	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 8.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LEU:HD22	1:A:605:LEU:HD21	1.44	0.97
1:B:331:LYS:HE3	1:B:361:PHE:HB3	1.65	0.79
1:B:283:ARG:HG3	1:B:309:CYS:SG	2.24	0.78
1:B:319:GLU:HG3	1:B:320:LEU:HD13	1.69	0.73
1:B:296:LEU:O	1:B:300:LEU:HD13	1.88	0.73
1:B:495:TYR:CE2	1:B:497:PRO:HG3	2.24	0.72
1:A:294:ALA:O	1:A:298:GLU:HG3	1.90	0.72
1:A:444:LYS:O	1:A:448:GLU:HG3	1.89	0.71
1:A:317:THR:HG21	4:A:1251:HOH:O	1.91	0.70
1:B:228:THR:OG1	1:B:249:ARG:HD2	1.92	0.69
1:B:409:ILE:HD12	1:B:618:HIS:CE1	2.28	0.68
1:B:114:VAL:HG11	1:B:158:LYS:HD2	1.76	0.67
1:A:4:TYR:HB2	1:A:306:SER:HB3	1.75	0.67
1:B:4:TYR:HB2	1:B:306:SER:HB3	1.76	0.66
1:B:448:GLU:O	1:B:452:GLU:HG3	1.95	0.66
1:B:511:THR:O	1:B:515:ILE:HG12	1.96	0.65
1:B:618:HIS:CE1	1:B:620:CYS:SG	2.90	0.65
1:B:501:TYR:O	1:B:543:ARG:HD2	1.96	0.65
1:B:711:TRP:O	1:B:715:ILE:HG12	1.97	0.64
1:A:409:ILE:HD11	1:A:704:CYS:HA	1.80	0.64
1:A:495:TYR:CE1	1:A:497:PRO:HG3	2.32	0.64
1:B:529:MET:HG3	4:B:1622:HOH:O	1.96	0.63
1:A:283:ARG:HG2	1:A:309:CYS:SG	2.39	0.63
1:B:679:ILE:HG23	1:B:724:LEU:HB2	1.81	0.62
1:A:665:GLY:HA2	1:A:699:TRP:HB2	1.82	0.61
1:B:228:THR:HG23	1:B:249:ARG:HG3	1.82	0.61
1:B:54:ASP:OD2	1:B:346:LYS:HE2	2.01	0.61
1:A:409:ILE:HD11	1:A:704:CYS:CA	2.31	0.60
1:B:665:GLY:HA2	1:B:699:TRP:HB2	1.83	0.60
1:B:543:ARG:HB3	1:B:545:ASP:OD1	2.02	0.60
1:B:331:LYS:HE2	1:B:364:PHE:CD2	2.37	0.60
1:B:691:ARG:HG3	1:B:692:VAL:HG23	1.84	0.60
1:A:557:LEU:CD2	1:A:605:LEU:HD21	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:NH1	1:B:572:LYS:HG2	2.17	0.59
1:A:678:SER:OG	1:A:681:GLU:HG3	2.02	0.59
1:A:201:PRO:O	1:A:204:VAL:HG22	2.03	0.59
1:A:47:GLU:HG3	4:A:853:HOH:O	2.02	0.58
1:B:509:PRO:HB3	1:B:512:LEU:HD12	1.86	0.58
1:A:32:GLU:O	1:A:36:GLU:HG3	2.04	0.58
1:B:560:ASN:OD1	1:B:564:LYS:HE2	2.04	0.57
1:A:563:VAL:O	1:A:567:GLU:HG3	2.04	0.57
1:A:232:TYR:O	1:A:233:TYR:HB2	2.05	0.57
1:A:15:ARG:HH21	1:A:15:ARG:HB2	1.69	0.56
1:A:512:LEU:HD11	1:A:565:ASP:HB3	1.86	0.56
1:B:232:TYR:O	1:B:233:TYR:HB2	2.06	0.56
1:A:696:GLU:H	1:A:696:GLU:CD	2.09	0.56
1:B:616:HIS:CE1	1:B:638:VAL:HG21	2.42	0.56
1:A:557:LEU:HD22	1:A:605:LEU:CD2	2.27	0.55
1:A:671:ILE:HD12	1:A:704:CYS:H	1.71	0.55
1:A:620:CYS:HB3	1:A:642:GLU:CD	2.27	0.55
1:B:512:LEU:HD11	1:B:565:ASP:HB3	1.87	0.55
1:B:714:VAL:O	1:B:718:LEU:HD13	2.07	0.55
1:B:87:LEU:HD22	1:B:91:PHE:CE1	2.42	0.54
1:A:509:PRO:HB3	1:A:512:LEU:HD12	1.90	0.54
1:B:571:ILE:HD12	1:B:571:ILE:N	2.22	0.54
1:A:671:ILE:HD13	4:A:1122:HOH:O	2.08	0.53
1:A:124:LEU:HD12	1:A:183:GLU:HG2	1.91	0.53
1:B:31:GLU:OE2	1:B:87:LEU:HB2	2.08	0.53
1:B:493:ARG:HD2	4:B:1477:HOH:O	2.08	0.53
1:B:509:PRO:CB	1:B:512:LEU:HD12	2.39	0.52
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.74	0.52
1:A:584:LYS:HG3	1:A:584:LYS:O	2.10	0.52
1:A:186:GLU:O	1:A:190:GLU:HG3	2.09	0.52
1:A:409:ILE:HD11	1:A:704:CYS:C	2.30	0.52
1:A:638:VAL:HG22	1:A:663:GLN:HB2	1.91	0.52
1:A:324:LEU:HD13	4:A:790:HOH:O	2.09	0.52
1:A:618:HIS:CE1	1:A:620:CYS:SG	3.03	0.52
1:B:240:GLU:HG3	4:B:1535:HOH:O	2.09	0.52
1:A:683:ARG:O	1:A:687:GLU:HG3	2.10	0.52
1:A:677:PRO:HB2	1:A:682:MET:CE	2.40	0.52
1:A:317:THR:HG22	1:A:319:GLU:H	1.75	0.51
1:A:231:THR:H	1:A:251:HIS:HD2	1.57	0.51
1:A:588:LYS:HD2	1:A:591:LYS:HE3	1.93	0.51
1:A:399:LEU:HB3	1:A:401:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:PRO:HG2	1:A:550:GLU:HB2	1.92	0.51
1:A:471:PHE:CZ	1:A:475:LYS:HE3	2.46	0.51
1:B:59:ASN:HB2	4:B:1486:HOH:O	2.09	0.51
1:B:701:ASN:HB2	1:B:702:PRO:HD2	1.92	0.50
1:A:270:PRO:HB2	1:A:273:LYS:HG2	1.94	0.50
1:B:288:VAL:O	1:B:290:LEU:HD22	2.11	0.50
1:A:368:LEU:C	1:A:368:LEU:HD13	2.32	0.50
1:A:671:ILE:HG13	1:A:705:GLY:O	2.12	0.50
1:B:399:LEU:HB3	1:B:401:LEU:HG	1.92	0.50
1:A:9:PRO:HB2	1:A:316:VAL:HG22	1.94	0.49
1:A:296:LEU:O	1:A:300:LEU:HD13	2.13	0.49
1:A:290:LEU:HD11	1:A:344:MET:HE3	1.95	0.49
1:B:715:ILE:HB	1:B:716:PRO:CD	2.43	0.49
1:B:686:VAL:O	1:B:689:VAL:HG22	2.13	0.49
1:B:696:GLU:H	1:B:696:GLU:CD	2.14	0.49
1:B:214:LEU:HD13	4:B:1526:HOH:O	2.13	0.49
1:B:477:ASN:HD21	1:B:507:PRO:HB3	1.78	0.48
1:B:272:ASP:OD1	1:B:273:LYS:HG3	2.12	0.48
1:A:2:LYS:HE2	1:A:55:VAL:CG2	2.44	0.48
1:A:409:ILE:C	1:A:409:ILE:HD12	2.34	0.47
1:A:707:LYS:HE2	4:A:1181:HOH:O	2.14	0.47
1:B:667:GLY:HA2	1:B:701:ASN:O	2.14	0.47
1:B:724:LEU:O	1:B:728:MET:HG2	2.13	0.47
1:B:563:VAL:O	1:B:567:GLU:HG3	2.15	0.47
1:B:201:PRO:O	1:B:204:VAL:HG22	2.14	0.47
1:A:582:ARG:HB3	1:A:621:TYR:CZ	2.50	0.47
1:A:546:ILE:HG13	1:A:547:PRO:HD2	1.97	0.47
1:B:620:CYS:HB3	1:B:642:GLU:CD	2.34	0.47
1:B:114:VAL:HG11	1:B:158:LYS:CD	2.45	0.46
1:A:589:LYS:O	1:B:168:ASN:HB3	2.15	0.46
1:A:671:ILE:HD12	1:A:704:CYS:N	2.31	0.46
1:A:677:PRO:HB2	1:A:682:MET:HE2	1.96	0.46
1:A:486:TRP:CE3	1:A:496:ARG:HG3	2.51	0.46
1:A:174:LEU:O	1:A:178:VAL:HG22	2.15	0.46
1:B:370:ALA:O	1:B:374:VAL:HG23	2.16	0.46
1:B:453:ILE:HG22	1:B:722:VAL:HG21	1.97	0.46
1:B:331:LYS:HE3	1:B:361:PHE:CB	2.41	0.46
1:B:319:GLU:HG3	1:B:320:LEU:CD1	2.43	0.46
1:A:707:LYS:HG2	1:A:707:LYS:O	2.16	0.46
1:A:178:VAL:HG21	1:A:221:GLU:OE2	2.15	0.46
1:A:712:ASP:OD1	1:A:713:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:HIS:NE2	1:A:620:CYS:SG	2.89	0.45
1:B:46:VAL:HG11	1:B:141:ILE:HD13	1.97	0.45
1:A:198:VAL:HG21	1:A:227:LEU:HG	1.97	0.45
1:B:564:LYS:O	1:B:568:GLU:HG3	2.16	0.45
1:B:471:PHE:CZ	1:B:475:LYS:HE3	2.51	0.45
1:A:589:LYS:HA	1:A:592:TRP:CD1	2.51	0.45
1:A:671:ILE:HD13	1:A:671:ILE:H	1.81	0.45
1:A:647:LYS:HD2	1:B:691:ARG:CZ	2.47	0.45
1:B:514:GLU:HG3	4:B:1554:HOH:O	2.17	0.45
1:B:370:ALA:HB3	1:B:503:THR:HG21	1.99	0.45
1:A:320:LEU:HD12	1:A:320:LEU:N	2.32	0.45
1:B:449:LEU:HD11	1:B:715:ILE:HD12	1.98	0.45
1:A:264:LEU:C	1:A:264:LEU:HD23	2.37	0.45
1:B:547:PRO:HG2	1:B:550:GLU:HB2	1.98	0.45
1:B:31:GLU:OE2	1:B:87:LEU:HD12	2.18	0.44
1:B:495:TYR:O	1:B:497:PRO:HD3	2.18	0.44
1:A:11:ILE:HA	1:A:17:PHE:HB3	1.99	0.44
1:B:669:TRP:CE3	1:B:702:PRO:HB3	2.52	0.44
1:B:324:LEU:HD13	4:B:1463:HOH:O	2.18	0.44
1:B:616:HIS:ND1	1:B:638:VAL:HG21	2.32	0.44
1:A:669:TRP:HZ3	1:A:718:LEU:HD13	1.82	0.44
1:B:158:LYS:HD3	4:B:1404:HOH:O	2.17	0.43
1:A:285:PRO:HD3	1:A:541:TYR:CD1	2.53	0.43
1:A:295:SER:O	1:A:299:LYS:HG3	2.18	0.43
1:B:644:SER:HB3	1:B:703:ASP:OD1	2.18	0.43
1:B:331:LYS:HE2	1:B:364:PHE:CG	2.54	0.43
1:B:68:LEU:HD22	1:B:113:LEU:CD1	2.48	0.43
1:B:341:GLU:HA	1:B:344:MET:CE	2.48	0.43
1:A:589:LYS:HG2	1:A:592:TRP:CZ2	2.53	0.43
1:A:457:VAL:HG22	1:A:525:PRO:HG2	2.00	0.43
1:B:616:HIS:CG	1:B:638:VAL:HG22	2.53	0.43
1:A:208:GLU:HA	1:B:208:GLU:HA	2.00	0.43
1:A:178:VAL:HG11	1:A:218:VAL:HG13	2.00	0.43
1:B:340:GLU:O	1:B:344:MET:HG3	2.18	0.43
1:A:72:VAL:O	1:A:125:LEU:HB3	2.18	0.43
1:B:128:LYS:N	1:B:129:PRO:CD	2.82	0.43
1:A:511:THR:O	1:A:515:ILE:HG12	2.19	0.43
1:B:477:ASN:O	1:B:504:VAL:HA	2.19	0.43
1:A:87:LEU:HD22	1:A:91:PHE:CE1	2.54	0.43
1:A:232:TYR:O	1:A:233:TYR:CB	2.67	0.42
1:B:231:THR:H	1:B:251:HIS:HD2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:HD23	4:A:1115:HOH:O	2.18	0.42
1:A:409:ILE:CD1	1:A:704:CYS:HA	2.49	0.42
1:B:566:LEU:O	1:B:571:ILE:HD13	2.19	0.42
1:B:341:GLU:HA	1:B:344:MET:HE2	2.01	0.42
1:B:5:ALA:HA	1:B:307:ASN:OD1	2.19	0.42
1:B:693:LEU:HA	1:B:694:PRO:HD3	1.93	0.42
1:B:477:ASN:ND2	1:B:507:PRO:HD3	2.34	0.41
1:B:236:VAL:HG21	1:B:252:PHE:HE2	1.85	0.41
1:B:446:ALA:O	1:B:450:GLN:HG3	2.21	0.41
1:A:10:LYS:HE2	1:A:488:LEU:HD22	2.02	0.41
1:B:220:ARG:HG2	1:B:220:ARG:HH21	1.86	0.41
1:A:644:SER:HA	1:A:685:ILE:HD13	2.01	0.41
1:B:232:TYR:O	1:B:233:TYR:CB	2.69	0.41
1:B:668:VAL:HG23	1:B:682:MET:CE	2.50	0.41
1:A:37:GLU:HA	1:A:40:LYS:HD3	2.03	0.41
1:A:651:ILE:O	1:A:655:GLU:HG2	2.20	0.41
1:B:409:ILE:HD12	1:B:618:HIS:HE1	1.82	0.41
1:B:724:LEU:HD13	1:B:724:LEU:C	2.41	0.41
1:B:459:VAL:HG12	1:B:527:LYS:HD3	2.01	0.41
1:A:384:ARG:HG3	1:A:635:GLU:OE1	2.20	0.41
1:A:403:LEU:HD11	1:A:695:LYS:HD2	2.03	0.40
1:B:17:PHE:O	1:B:21:LEU:HD13	2.21	0.40
1:B:726:LYS:O	1:B:730:GLU:HG3	2.20	0.40
1:B:46:VAL:HG21	1:B:136:PHE:CE2	2.57	0.40
1:A:411:SER:HB2	1:A:707:LYS:HB2	2.04	0.40
1:A:669:TRP:CD1	1:A:677:PRO:HG2	2.56	0.40
1:A:59:ASN:HB2	4:A:820:HOH:O	2.20	0.40
1:B:228:THR:OG1	1:B:249:ARG:CD	2.66	0.40
1:A:178:VAL:CG1	1:A:218:VAL:HG13	2.52	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	732/766 (96%)	703 (96%)	28 (4%)	1 (0%)	56 53
1	B	727/766 (95%)	696 (96%)	29 (4%)	2 (0%)	46 41
All	All	1459/1532 (95%)	1399 (96%)	57 (4%)	3 (0%)	52 48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	TYR
1	B	233	TYR
1	B	64	TYR

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	608/688 (88%)	583 (96%)	25 (4%)	37 32
1	B	595/688 (86%)	580 (98%)	15 (2%)	55 55
All	All	1203/1376 (87%)	1163 (97%)	40 (3%)	45 43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	32	GLU
1	A	47	GLU
1	A	85	ARG
1	A	124	LEU
1	A	154	LEU
1	A	227	LEU
1	A	245	LEU
1	A	251	HIS
1	A	285	PRO
1	A	312	PHE
1	A	317	THR
1	A	323	ASN

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	339	LEU
1	A	369	GLN
1	A	399	LEU
1	A	403	LEU
1	A	493	ARG
1	A	529	MET
1	A	557	LEU
1	A	671	ILE
1	A	701	ASN
1	A	704	CYS
1	A	718	LEU
1	B	154	LEU
1	B	245	LEU
1	B	285	PRO
1	B	324	LEU
1	B	339	LEU
1	B	398	ARG
1	B	399	LEU
1	B	403	LEU
1	B	458	LEU
1	B	476	LEU
1	B	488	LEU
1	B	529	MET
1	B	557	LEU
1	B	582	ARG
1	B	638	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	A	323	ASN
1	A	369	GLN
1	A	400	ASN
1	A	710	ASN
1	B	251	HIS
1	B	267	HIS
1	B	323	ASN
1	B	477	ASN
1	B	601	ASN
1	B	625	ASN

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Mol	Chain	Res	Type
1	B	710	ASN

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	SO4	A	1350	-	4,4,4	0.12	0	6,6,6	0.07	0
3	MRY	A	1353	-	7,7,7	0.29	0	6,8,8	0.47	0
2	SO4	B	1351	-	4,4,4	0.09	0	6,6,6	0.11	0
3	MRY	B	1352	-	7,7,7	0.28	0	6,8,8	0.50	0

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	SO4	A	1350	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MRY	A	1353	-	-	0/8/8/8	0/0/0/0
2	SO4	B	1351	-	-	0/0/0/0	0/0/0/0
3	MRY	B	1352	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	734/766 (95%)	0.11	25 (3%) 49 50	12, 25, 43, 58	0
1	B	731/766 (95%)	0.22	32 (4%) 38 39	13, 26, 46, 68	0
All	All	1465/1532 (95%)	0.17	57 (3%) 43 45	12, 25, 45, 68	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	PHE	8.2
1	B	428	GLY	6.4
1	B	377	LEU	5.1
1	B	674	PRO	4.8
1	B	359	VAL	4.6
1	B	362	GLU	4.3
1	B	425	TYR	4.0
1	B	431	SER	3.9
1	A	704	CYS	3.9
1	A	672	HIS	3.9
1	A	732	PHE	3.9
1	A	377	LEU	3.8
1	A	380	ASP	3.7
1	B	620	CYS	3.5
1	A	427	LYS	3.5
1	A	381	SER	3.4
1	B	-1	PRO	3.4
1	B	368	LEU	3.3
1	A	428	GLY	3.2
1	B	705	GLY	3.1
1	A	351	GLY	3.1
1	A	358	ASN	3.0
1	B	363	ASP	3.0
1	B	360	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	672	HIS	2.9
1	A	426	ARG	2.9
1	B	423	SER	2.8
1	A	0	PHE	2.8
1	B	416	PRO	2.7
1	A	373	ARG	2.7
1	B	427	LYS	2.7
1	B	415	THR	2.7
1	B	675	ALA	2.6
1	A	620	CYS	2.5
1	B	730	GLU	2.5
1	B	622	SER	2.5
1	B	272	ASP	2.5
1	A	356	LEU	2.5
1	A	352	LYS	2.4
1	A	671	ILE	2.3
1	A	705	GLY	2.3
1	A	706	LEU	2.3
1	A	378	PRO	2.3
1	B	679	ILE	2.2
1	A	623	ASP	2.2
1	A	733	GLU	2.2
1	B	-2	ASP	2.2
1	B	545	ASP	2.1
1	B	673	SER	2.1
1	A	674	PRO	2.1
1	B	610	ARG	2.1
1	B	96	GLY	2.1
1	A	668	VAL	2.1
1	B	546	ILE	2.1
1	B	520	SER	2.1
1	B	569	ALA	2.0
1	A	361	PHE	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	MRY	A	1353	8/8	0.90	0.19	3.38	24,37,39,42	0
3	MRY	B	1352	8/8	0.93	0.15	1.35	23,34,36,39	0
2	SO4	B	1351	5/5	0.99	0.10	-0.89	24,25,27,29	0
2	SO4	A	1350	5/5	0.99	0.08	-1.73	26,27,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.