Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:17 PM GMT

PDB ID	:	3THR
Title	:	Crystal structure of rat native liver Glycine N-methyltransferase complexed with 5-methyltetrahydrofolate monoglutamate
Authors	:	Luka, Z.; Pakhomova, S.; Loukachevitch, L.V.; Newcomer, M.E.; Wagner, C.
Deposited on	:	2011-08-19
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:

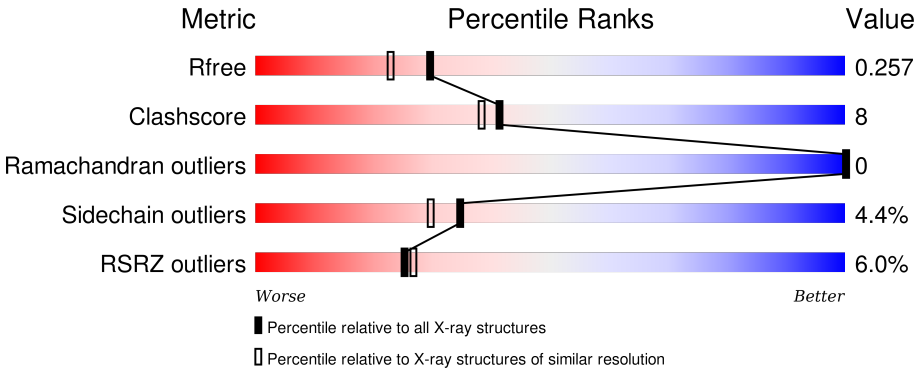
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	293	6% 83% 13%
1	B	293	6% 82% 14%
1	C	293	6% 85% 11%
1	D	293	4% 84% 11%

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	C2F	A	1100	-	-	X	X
2	C2F	B	1700	-	-	-	X
2	C2F	D	1200	-	-	X	X
3	TAM	A	1500	-	-	-	X
3	TAM	C	1600	-	-	-	X
3	TAM	D	1400	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9887 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.

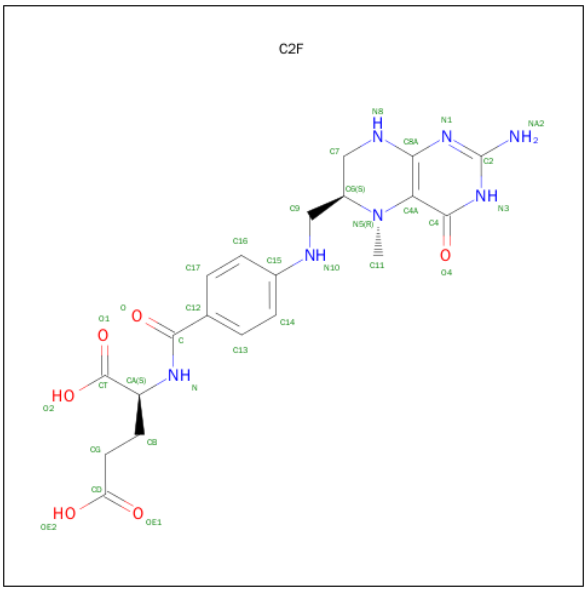
- Molecule 1 is a protein called Glycine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2255	1435	390	419	11			
1	B	287	Total	C	N	O	S	0	0	0
			2249	1430	390	418	11			
1	C	285	Total	C	N	O	S	0	2	0
			2250	1432	390	417	11			
1	D	286	Total	C	N	O	S	0	0	0
			2243	1428	388	416	11			

There are 4 discrepancies between the modelled and reference sequences:

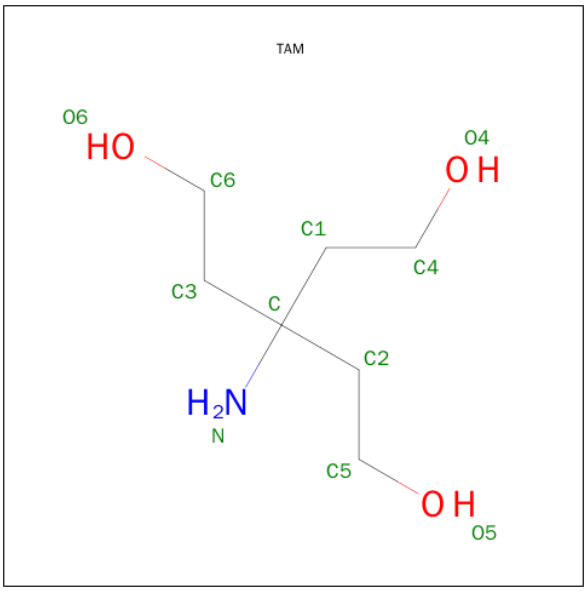
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	ACE	-	ACETYLATION	UNP P13255
B	300	ACE	-	ACETYLATION	UNP P13255
C	300	ACE	-	ACETYLATION	UNP P13255
D	300	ACE	-	ACETYLATION	UNP P13255

- Molecule 2 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (three-letter code: C2F) (formula: $C_{20}H_{25}N_7O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 33 20 7 6	0	0
2	B	1	Total C N O 33 20 7 6	0	0
2	C	1	Total C N O 33 20 7 6	0	0
2	D	1	Total C N O 33 20 7 6	0	0

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	C	1	Total	C	N	O	0	0
			11	7	1	3		
3	D	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is water.

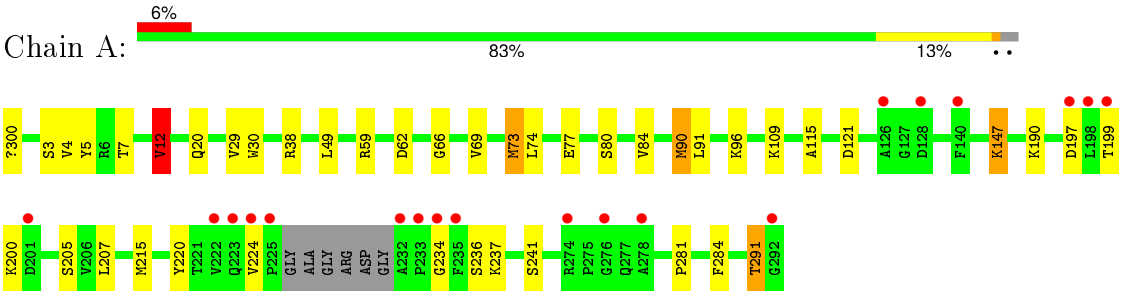
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	161	Total	O	0	0
			161	161		
4	C	248	Total	O	0	0
			248	248		
4	D	181	Total	O	0	0
			181	181		

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.

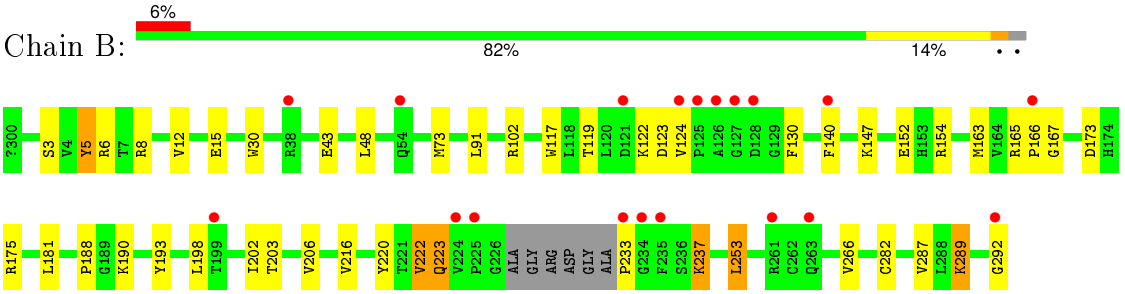
- Molecule 1: Glycine N-methyltransferase

Chain A:



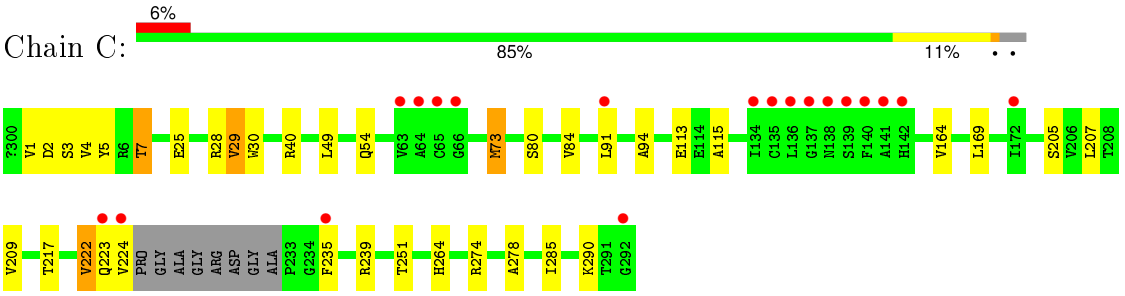
- Molecule 1: Glycine N-methyltransferase

Chain B:



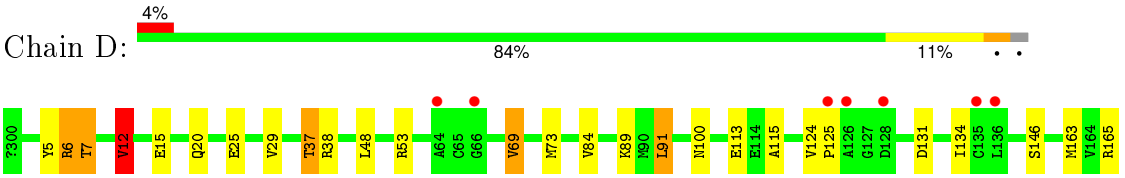
- Molecule 1: Glycine N-methyltransferase

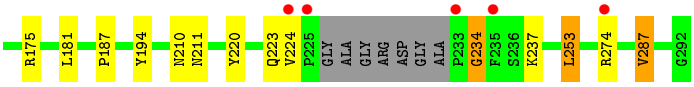
Chain C:



- Molecule 1: Glycine N-methyltransferase

Chain D:




R175
L181
P187
Y194
N210
N211
Y220
Q223
V224
P225
GLY
ALA
GLY
ARG
ASP
GLY
ALA
P233
G234
F235
S236
K237
L253
R274
V287
G292

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.19Å 83.79Å 134.44Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	31.19 – 2.00 31.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.1 (31.19-2.00) 87.1 (31.19-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.241 0.200 , 0.257	Depositor DCC
R_{free} test set	4037 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.7	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 83611 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9887	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: TAM, C2F, ACE

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	0.98	0/2311	0.92	4/3134 (0.1%)
1	B	1.01	4/2301 (0.2%)	0.94	3/3119 (0.1%)
1	C	1.15	6/2309 (0.3%)	1.00	11/3129 (0.4%)
1	D	1.14	1/2296 (0.0%)	1.00	8/3113 (0.3%)
All	All	1.08	11/9217 (0.1%)	0.97	26/12495 (0.2%)

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	A	0	1
1	D	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	TYR	CD1-CE1	-7.81	1.27	1.39
1	B	5	TYR	CD2-CE2	-7.72	1.27	1.39
1	B	5	TYR	CD1-CE1	-7.01	1.28	1.39
1	C	94	ALA	CA-CB	6.54	1.66	1.52
1	C	278	ALA	CA-CB	5.69	1.64	1.52
1	C	5	TYR	CD2-CE2	-5.58	1.30	1.39
1	C	209	VAL	CB-CG2	5.42	1.64	1.52
1	B	43	GLU	CG-CD	5.39	1.60	1.51
1	D	287	VAL	CA-CB	5.32	1.66	1.54
1	B	152	GLU	CG-CD	5.30	1.59	1.51
1	C	25	GLU	CD-OE2	5.13	1.31	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	40	ARG	NE-CZ-NH1	-8.45	116.07	120.30
1	C	274	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	C	73	MET	CG-SD-CE	-7.77	87.77	100.20
1	D	91	LEU	CB-CG-CD1	7.08	123.03	111.00
1	C	28	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	233	PRO	N-CA-CB	6.25	110.79	103.30
1	C	91	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	121	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	274	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	12	VAL	CG1-CB-CG2	5.99	120.47	110.90
1	D	6	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	12	VAL	CG1-CB-CG2	5.86	120.27	110.90
1	C	29	VAL	CB-CA-C	-5.85	100.28	111.40
1	D	53	ARG	CG-CD-NE	5.84	124.07	111.80
1	B	253	LEU	CA-CB-CG	5.69	128.40	115.30
1	D	175	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	59	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	154	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	62	ASP	CB-CG-OD1	5.42	123.17	118.30
1	C	40	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	D	53	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	239	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	169	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	131	ASP	CB-CG-OD2	5.08	122.88	118.30
1	D	175	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	285	ILE	CG1-CB-CG2	-5.02	100.36	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	THR	Peptide
1	D	234	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2255	0	2217	46	0
1	B	2249	0	2205	36	0
1	C	2250	0	2213	25	0
1	D	2243	0	2202	44	0
2	A	33	0	23	21	0
2	B	33	0	23	2	0
2	C	33	0	23	2	0
2	D	33	0	22	18	0
3	A	11	0	17	5	0
3	C	11	0	17	4	0
3	D	11	0	17	3	0
4	A	135	0	0	5	0
4	B	161	0	0	2	0
4	C	248	0	0	4	0
4	D	181	0	0	10	0
All	All	9887	0	8979	154	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 (154) 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)
3:C:1600:TAM:C6	3:C:1600:TAM:O6	1.71	1.36
1:A:5:TYR:CZ	2:A:1100:C2F:HB1	1.82	1.12
1:D:37:THR:CG2	1:D:69:VAL:HG21	1.80	1.12
1:D:5:TYR:CZ	2:D:1200:C2F:HB1	1.94	1.02
1:A:49:LEU:HD21	1:A:73:MET:HE3	1.51	0.92
1:B:223:GLN:HE21	1:B:223:GLN:H	1.11	0.91
1:C:29:VAL:CG1	1:C:222:VAL:HG22	2.02	0.90
1:D:37:THR:HG21	1:D:69:VAL:HG21	1.52	0.89
1:B:3:SER:CB	2:D:1200:C2F:O4	2.20	0.88
1:A:49:LEU:HD21	1:A:73:MET:CE	2.04	0.86
1:D:37:THR:HG23	1:D:69:VAL:HG21	1.54	0.86
1:A:5:TYR:HB3	2:A:1100:C2F:C17	2.07	0.84
1:B:223:GLN:HE21	1:B:223:GLN:N	1.76	0.82
1:A:5:TYR:HB3	2:A:1100:C2F:H17	1.62	0.80
1:A:5:TYR:CB	2:A:1100:C2F:H17	2.12	0.80
1:A:5:TYR:CZ	2:A:1100:C2F:CB	2.63	0.79
1:C:29:VAL:CG1	1:C:222:VAL:CG2	2.62	0.77
2:C:1410:C2F:HA	2:C:1410:C2F:OE2	1.84	0.77
1:A:12:VAL:HG22	1:B:30:TRP:CG	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:TYR:HB3	2:D:1200:C2F:C17	2.14	0.77
1:A:49:LEU:CD2	1:A:73:MET:CE	2.63	0.76
1:B:166:PRO:HA	1:B:292:GLY:HA2	1.68	0.73
1:B:223:GLN:NE2	1:B:223:GLN:H	1.86	0.73
1:A:49:LEU:CD2	1:A:73:MET:HE3	2.17	0.73
2:A:1100:C2F:O4	1:C:3:SER:HB2	1.89	0.72
1:C:29:VAL:HG11	1:C:222:VAL:HG22	1.71	0.72
3:C:1600:TAM:H51	4:C:519:HOH:O	1.91	0.71
1:C:2:ASP:HA	4:C:705:HOH:O	1.90	0.70
1:A:5:TYR:CE2	2:A:1100:C2F:HB2	2.27	0.70
1:A:30:TRP:CG	1:B:12:VAL:HG22	2.27	0.69
1:A:5:TYR:CE2	2:A:1100:C2F:CB	2.76	0.69
1:A:7:THR:CG2	2:A:1100:C2F:H113	2.22	0.69
2:A:1100:C2F:O4	2:A:1100:C2F:C11	2.40	0.68
1:B:3:SER:HB3	2:D:1200:C2F:O4	1.93	0.68
1:A:73:MET:HE1	1:A:74:LEU:HD23	1.76	0.68
1:C:2:ASP:OD2	4:C:705:HOH:O	2.12	0.67
1:B:48:LEU:HD23	1:B:73:MET:HE1	1.77	0.66
1:A:49:LEU:CD2	1:A:73:MET:HE1	2.26	0.65
2:A:1100:C2F:O4	1:C:3:SER:CB	2.45	0.64
1:B:3:SER:HB2	2:D:1200:C2F:O4	1.96	0.64
1:A:7:THR:HG22	2:A:1100:C2F:H113	1.80	0.63
1:D:5:TYR:CB	2:D:1200:C2F:H17	2.29	0.62
1:A:5:TYR:OH	2:A:1100:C2F:HB1	1.99	0.62
1:D:5:TYR:CE2	2:D:1200:C2F:HB1	2.35	0.61
1:D:5:TYR:CZ	2:D:1200:C2F:CB	2.79	0.61
1:D:5:TYR:CE2	2:D:1200:C2F:CB	2.85	0.60
1:D:224:VAL:HB	4:D:543:HOH:O	2.02	0.60
1:C:30:TRP:CG	1:D:12:VAL:HG22	2.37	0.59
1:A:49:LEU:HD23	1:A:73:MET:HE1	1.84	0.59
1:D:100:ASN:ND2	4:D:380:HOH:O	2.35	0.59
1:B:206:VAL:HG22	1:B:216:VAL:HG22	1.85	0.59
1:A:84:VAL:HG13	1:A:115:ALA:HB3	1.84	0.58
1:C:251:THR:HG23	1:C:264:HIS:CE1	2.38	0.58
1:D:5:TYR:CB	2:D:1200:C2F:C17	2.81	0.58
1:D:187:PRO:HD2	4:D:584:HOH:O	2.01	0.58
2:B:1700:C2F:O2	2:B:1700:C2F:HG1	2.04	0.57
1:D:38:ARG:NH2	4:D:603:HOH:O	2.37	0.57
1:B:48:LEU:HD23	1:B:73:MET:CE	2.34	0.57
1:B:198:LEU:HD11	1:B:222:VAL:HG21	1.88	0.56
1:C:29:VAL:HG13	1:C:222:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD21	1:C:73:MET:HE1	1.88	0.56
1:C:29:VAL:HG13	1:C:222:VAL:HG22	1.87	0.56
3:A:1500:TAM:H12	1:B:15:GLU:OE2	2.05	0.55
1:D:5:TYR:OH	2:D:1200:C2F:HB1	2.05	0.54
1:B:6:ARG:NH1	1:B:8:ARG:O	2.38	0.53
1:B:175:ARG:NE	4:B:567:HOH:O	2.31	0.53
1:A:109:LYS:HE2	4:A:565:HOH:O	2.08	0.53
1:D:37:THR:HG22	4:D:714:HOH:O	2.09	0.53
1:A:5:TYR:CG	2:A:1100:C2F:H17	2.43	0.53
2:C:1410:C2F:CD	2:C:1410:C2F:O	2.56	0.53
1:B:130:PHE:O	1:B:165:ARG:HG2	2.09	0.53
1:B:202:ILE:HD13	4:B:542:HOH:O	2.08	0.53
1:A:3:SER:O	1:C:7:THR:HG23	2.10	0.52
1:C:217:THR:OG1	2:D:1200:C2F:H14	2.11	0.51
1:D:69:VAL:HG13	1:D:194:TYR:CZ	2.45	0.51
1:D:5:TYR:CE2	2:D:1200:C2F:HB2	2.46	0.51
1:D:69:VAL:HG13	1:D:194:TYR:OH	2.10	0.51
3:A:1500:TAM:H12	1:B:15:GLU:CD	2.30	0.51
3:D:1400:TAM:H31	4:D:444:HOH:O	2.11	0.51
1:C:29:VAL:CG1	1:C:222:VAL:HG21	2.40	0.50
1:A:5:TYR:CE2	2:A:1100:C2F:HB1	2.36	0.50
1:B:188:PRO:HB3	1:B:202:ILE:HD12	1.94	0.50
1:A:281:PRO:HG2	1:A:284:PHE:CE1	2.48	0.49
1:A:7:THR:HG23	1:C:3:SER:O	2.11	0.49
1:A:5:TYR:CE1	2:A:1100:C2F:CT	2.96	0.49
2:B:1700:C2F:O2	2:B:1700:C2F:CG	2.61	0.48
1:D:48:LEU:HD23	1:D:73:MET:CE	2.43	0.48
1:B:147:LYS:O	1:B:147:LYS:HG3	2.13	0.48
1:A:5:TYR:HB3	2:A:1100:C2F:C16	2.42	0.48
1:A:66:GLY:HA2	1:A:90:MET:HG2	1.96	0.47
1:A:220:TYR:O	1:A:237:LYS:HA	2.14	0.47
3:A:1500:TAM:H21	1:B:15:GLU:OE1	2.14	0.47
1:B:3:SER:O	1:D:7:THR:HG23	2.14	0.47
1:D:223:GLN:HA	1:D:234:GLY:O	2.15	0.47
1:D:89:LYS:NZ	4:D:354:HOH:O	2.48	0.47
3:A:1500:TAM:C5	4:A:487:HOH:O	2.63	0.47
1:B:222:VAL:CG1	1:B:223:GLN:N	2.78	0.46
1:D:84:VAL:HA	1:D:113:GLU:O	2.16	0.46
1:D:5:TYR:CG	2:D:1200:C2F:H17	2.50	0.46
1:D:100:ASN:ND2	4:D:341:HOH:O	2.49	0.46
1:D:25:GLU:O	1:D:29:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD13	4:D:570:HOH:O	2.15	0.45
1:A:147:LYS:HE2	4:A:666:HOH:O	2.17	0.45
1:A:5:TYR:CB	2:A:1100:C2F:C17	2.80	0.45
1:A:20:GLN:HG2	4:C:705:HOH:O	2.17	0.45
2:A:1100:C2F:O4	2:A:1100:C2F:H113	2.15	0.44
1:A:207:LEU:HD11	1:C:205:SER:HB3	1.98	0.44
1:D:220:TYR:O	1:D:237:LYS:HA	2.17	0.44
1:B:167:GLY:O	1:B:289:LYS:HD2	2.17	0.44
3:C:1600:TAM:H61	1:D:15:GLU:OE1	2.17	0.44
1:C:84:VAL:HA	1:C:113:GLU:O	2.18	0.44
1:B:124:VAL:CG1	1:B:163:MET:HE1	2.48	0.44
1:D:7:THR:HG22	2:D:1200:C2F:H92	2.00	0.44
1:B:220:TYR:O	1:B:237:LYS:HA	2.18	0.44
1:B:119:THR:OG1	1:B:123:ASP:OD1	2.35	0.44
1:D:20:GLN:HG3	4:D:307:HOH:O	2.17	0.44
1:D:7:THR:CG2	2:D:1200:C2F:H113	2.48	0.43
1:A:300:ACE:H2	1:D:146:SER:HB3	2.01	0.43
1:A:73:MET:HE3	1:A:77:GLU:HG3	2.00	0.43
1:A:4:VAL:HG22	4:A:558:HOH:O	2.19	0.43
1:A:12:VAL:HG22	1:B:30:TRP:CD2	2.53	0.43
1:C:164:VAL:HB	1:C:290:LYS:HE3	2.00	0.43
1:D:224:VAL:O	1:D:234:GLY:CA	2.67	0.43
1:D:134:ILE:HG13	1:D:134:ILE:O	2.19	0.43
1:C:4:VAL:O	1:C:4:VAL:HG23	2.19	0.42
1:D:5:TYR:HB3	2:D:1200:C2F:C16	2.49	0.42
1:A:73:MET:CE	1:A:74:LEU:HD23	2.47	0.42
1:D:48:LEU:HD23	1:D:73:MET:HE1	1.99	0.42
1:D:37:THR:O	1:D:37:THR:CG2	2.68	0.42
1:A:30:TRP:CD2	1:B:12:VAL:HG22	2.55	0.42
1:B:203:THR:HG23	1:D:210:ASN:ND2	2.33	0.42
1:D:124:VAL:HA	1:D:125:PRO:HD2	1.89	0.42
1:C:223:GLN:HB2	1:C:235:PHE:CE1	2.55	0.42
1:B:173:ASP:OD2	1:B:193:TYR:OH	2.31	0.42
1:B:190:LYS:HE2	1:B:282:CYS:SG	2.60	0.41
2:A:1100:C2F:O4	2:A:1100:C2F:H112	2.19	0.41
3:A:1500:TAM:H51	4:A:487:HOH:O	2.19	0.41
3:C:1600:TAM:C6	3:C:1600:TAM:HO6	2.14	0.41
1:B:5:TYR:HD1	2:D:1200:C2F:N8	2.18	0.41
1:A:224:VAL:O	1:A:234:GLY:N	2.53	0.41
1:C:84:VAL:HB	1:C:115:ALA:HB3	2.02	0.41
1:A:29:VAL:HG21	1:A:236:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HE3	1:A:241:SER:OG	2.20	0.41
1:A:84:VAL:CG1	1:A:115:ALA:HB3	2.50	0.41
1:A:96:LYS:HB2	1:A:96:LYS:HE2	1.96	0.41
1:A:205:SER:HB3	1:C:207:LEU:HD11	2.03	0.41
1:C:29:VAL:HG12	1:C:222:VAL:HG21	2.03	0.41
3:D:1400:TAM:HN1	3:D:1400:TAM:H41	1.41	0.41
1:D:84:VAL:HB	1:D:115:ALA:HB3	2.03	0.41
1:D:124:VAL:HG12	1:D:163:MET:HE1	2.02	0.41
2:A:1100:C2F:O4	1:C:3:SER:HB3	2.19	0.40
1:B:166:PRO:CA	1:B:292:GLY:HA2	2.47	0.40
1:B:117:TRP:CH2	1:B:140:PHE:HA	2.57	0.40
3:D:1400:TAM:H61	3:D:1400:TAM:HN2	0.96	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	284/293 (97%)	279 (98%)	5 (2%)	0	100	100
1	B	283/293 (97%)	277 (98%)	6 (2%)	0	100	100
1	C	283/293 (97%)	272 (96%)	11 (4%)	0	100	100
1	D	282/293 (96%)	272 (96%)	10 (4%)	0	100	100
All	All	1132/1172 (97%)	1100 (97%)	32 (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	241/242 (100%)	228 (95%)	13 (5%)	27	21
1	B	239/242 (99%)	228 (95%)	11 (5%)	33	28
1	C	241/242 (100%)	234 (97%)	7 (3%)	50	49
1	D	239/242 (99%)	227 (95%)	12 (5%)	30	24
All	All	960/968 (99%)	917 (96%)	43 (4%)	35	29

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	38	ARG
1	A	69	VAL
1	A	73	MET
1	A	80	SER
1	A	90	MET
1	A	91	LEU
1	A	147	LYS
1	A	190	LYS
1	A	197	ASP
1	A	199	THR
1	A	200	LYS
1	A	291	THR
1	B	91	LEU
1	B	102	ARG
1	B	122	LYS
1	B	181	LEU
1	B	222	VAL
1	B	223	GLN
1	B	237	LYS
1	B	253	LEU
1	B	266	VAL
1	B	287	VAL
1	B	289	LYS
1	C	1	VAL
1	C	7	THR
1	C	54	GLN
1	C	80[A]	SER

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Mol	Chain	Res	Type
1	C	80[B]	SER
1	C	222	VAL
1	C	224	VAL
1	D	6	ARG
1	D	7	THR
1	D	12	VAL
1	D	37	THR
1	D	69	VAL
1	D	91	LEU
1	D	165	ARG
1	D	181	LEU
1	D	211	ASN
1	D	253	LEU
1	D	274	ARG
1	D	287	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	B	100	ASN
1	B	211	ASN
1	B	223	GLN
1	C	54	GLN
1	C	100	ASN
1	C	150	GLN
1	C	210	ASN
1	C	214	HIS
1	C	223	GLN
1	D	100	ASN
1	D	159	ASN
1	D	211	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)

7 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	C2F	A	1100	-	25,35,35	1.60	4 (16%)	27,49,49	2.53	14 (51%)
3	TAM	A	1500	-	7,10,10	1.51	1 (14%)	9,12,12	6.25	6 (66%)
2	C2F	B	1700	-	25,35,35	1.15	2 (8%)	27,49,49	2.00	8 (29%)
2	C2F	C	1410	-	25,35,35	0.85	1 (4%)	27,49,49	1.96	8 (29%)
3	TAM	C	1600	-	7,10,10	3.18	5 (71%)	9,12,12	4.09	6 (66%)
2	C2F	D	1200	-	25,35,35	1.45	6 (24%)	27,49,49	2.17	13 (48%)
3	TAM	D	1400	-	7,10,10	1.87	2 (28%)	9,12,12	4.76	5 (55%)

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	C2F	A	1100	-	-	0/16/35/35	0/3/3/3
3	TAM	A	1500	-	-	0/12/12/12	0/0/0/0
2	C2F	B	1700	-	-	0/16/35/35	0/3/3/3
2	C2F	C	1410	-	-	0/16/35/35	0/3/3/3
3	TAM	C	1600	-	-	0/12/12/12	0/0/0/0
2	C2F	D	1200	-	-	0/16/35/35	0/3/3/3
3	TAM	D	1400	-	-	0/12/12/12	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	C2F	C16-C15	-3.87	1.32	1.39
2	A	1100	C2F	C17-C12	-3.32	1.33	1.39
2	D	1200	C2F	C-N	-2.19	1.29	1.34
2	B	1700	C2F	C2-NA2	2.04	1.38	1.34
2	D	1200	C2F	C8A-N1	2.06	1.38	1.34
3	C	1600	TAM	C1-C4	2.08	1.56	1.52
2	D	1200	C2F	C2-N1	2.10	1.39	1.35
2	B	1700	C2F	C8A-N1	2.42	1.39	1.34
2	D	1200	C2F	C2-NA2	2.46	1.39	1.34
2	A	1100	C2F	C8A-N1	2.47	1.39	1.34
3	C	1600	TAM	O4-C4	2.47	1.55	1.42
2	D	1200	C2F	CB-CA	2.52	1.56	1.53
3	D	1400	TAM	C2-C5	2.54	1.57	1.52
2	C	1410	C2F	CA-N	2.59	1.50	1.46
3	A	1500	TAM	C2-C5	2.84	1.58	1.52
2	A	1100	C2F	C7-N8	2.84	1.49	1.46
2	D	1200	C2F	C6-N5	2.99	1.50	1.47
3	C	1600	TAM	O5-C5	3.29	1.59	1.42
3	D	1400	TAM	C3-C6	3.43	1.59	1.52
3	C	1600	TAM	C3-C6	4.33	1.61	1.52
3	C	1600	TAM	O6-C6	5.51	1.71	1.42

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1500	TAM	C3-C-C1	-11.40	92.29	110.50
3	D	1400	TAM	C3-C-N	-7.33	93.14	108.28
3	A	1500	TAM	O6-C6-C3	-6.36	96.65	111.14
3	A	1500	TAM	C3-C-C2	-5.60	101.55	110.50
2	A	1100	C2F	C14-C13-C12	-4.45	115.60	120.76
2	A	1100	C2F	N3-C2-N1	-4.42	118.28	125.53
2	B	1700	C2F	C12-C-N	-3.82	110.13	116.93
2	D	1200	C2F	C12-C-N	-3.74	110.27	116.93
2	C	1410	C2F	N3-C2-N1	-3.67	119.51	125.53
2	D	1200	C2F	N3-C2-N1	-3.60	119.63	125.53
2	B	1700	C2F	N3-C2-N1	-3.54	119.73	125.53
2	A	1100	C2F	C12-C-N	-3.43	110.83	116.93
2	C	1410	C2F	C4A-C4-N3	-3.35	118.31	123.46
2	D	1200	C2F	C14-C13-C12	-3.22	117.03	120.76
2	A	1100	C2F	C17-C12-C	-3.18	110.51	120.60
3	C	1600	TAM	C1-C-N	-3.02	102.03	108.28
3	C	1600	TAM	C2-C-C1	-2.98	105.75	110.50
2	B	1700	C2F	C4A-C4-N3	-2.52	119.59	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1200	C2F	C17-C12-C	-2.30	113.30	120.60
3	D	1400	TAM	C1-C-N	-2.22	103.68	108.28
2	C	1410	C2F	O-C-C12	-2.11	117.37	120.97
2	C	1410	C2F	NA2-C2-N3	2.03	120.56	117.20
2	D	1200	C2F	C13-C12-C	2.04	127.07	120.60
2	B	1700	C2F	O-C-N	2.08	126.19	122.44
2	D	1200	C2F	O-C-C12	2.30	124.90	120.97
2	C	1410	C2F	C2-N1-C8A	2.30	119.70	114.54
2	D	1200	C2F	C16-C17-C12	2.33	123.46	120.76
2	B	1700	C2F	C2-N1-C8A	2.36	119.85	114.54
2	A	1100	C2F	C13-C14-C15	2.38	122.96	120.28
2	A	1100	C2F	C2-N1-C8A	2.40	119.92	114.54
2	A	1100	C2F	CG-CB-CA	2.40	117.86	112.99
2	D	1200	C2F	C13-C14-C15	2.42	123.00	120.28
2	A	1100	C2F	O-C-C12	2.48	125.21	120.97
2	D	1200	C2F	C4-C4A-C8A	2.59	116.50	114.43
2	B	1700	C2F	NA2-C2-N1	2.64	121.58	117.20
2	D	1200	C2F	C4-N3-C2	2.71	119.69	115.94
2	A	1100	C2F	C13-C12-C	2.77	129.40	120.60
2	D	1200	C2F	C2-N1-C8A	2.81	120.86	114.54
2	A	1100	C2F	C9-N10-C15	2.96	128.93	121.46
2	A	1100	C2F	C16-C17-C12	3.03	124.27	120.76
2	C	1410	C2F	C12-C-N	3.09	122.44	116.93
3	C	1600	TAM	O5-C5-C2	3.18	118.40	111.14
2	C	1410	C2F	C4-C4A-C8A	3.35	117.09	114.43
2	D	1200	C2F	NA2-C2-N1	3.54	123.06	117.20
3	A	1500	TAM	O5-C5-C2	3.57	119.29	111.14
2	A	1100	C2F	C4-C4A-C8A	3.64	117.33	114.43
2	D	1200	C2F	CG-CB-CA	4.10	121.32	112.99
2	A	1100	C2F	C4-N3-C2	4.12	121.66	115.94
3	D	1400	TAM	O4-C4-C1	4.29	120.94	111.14
2	B	1700	C2F	C4-N3-C2	4.51	122.20	115.94
2	B	1700	C2F	C4-C4A-C8A	4.83	118.27	114.43
2	A	1100	C2F	NA2-C2-N1	4.85	125.22	117.20
2	C	1410	C2F	C4-N3-C2	5.00	122.88	115.94
3	A	1500	TAM	C2-C-N	5.00	118.61	108.28
3	C	1600	TAM	C3-C-C1	5.13	118.70	110.50
3	C	1600	TAM	O4-C4-C1	5.24	123.09	111.14
3	D	1400	TAM	O5-C5-C2	5.39	123.44	111.14
3	C	1600	TAM	O6-C6-C3	7.85	129.04	111.14
3	D	1400	TAM	C2-C-C1	9.48	125.65	110.50
3	A	1500	TAM	C2-C-C1	10.31	126.97	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	C2F	21	0
3	A	1500	TAM	5	0
2	B	1700	C2F	2	0
2	C	1410	C2F	2	0
3	C	1600	TAM	4	0
2	D	1200	C2F	18	0
3	D	1400	TAM	3	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	286/293 (97%)	0.44	19 (6%)	22	22	4, 15, 30, 38	0
1	B	286/293 (97%)	0.40	19 (6%)	22	22	8, 17, 32, 43	0
1	C	284/293 (96%)	0.33	19 (6%)	21	22	3, 16, 28, 46	0
1	D	285/293 (97%)	0.28	12 (4%)	40	41	9, 17, 33, 46	0
All	All	1141/1172 (97%)	0.36	69 (6%)	25	27	3, 16, 31, 46	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	ALA	7.5
1	B	128	ASP	6.1
1	A	224	VAL	5.9
1	A	232	ALA	5.7
1	B	125	PRO	5.7
1	A	233	PRO	5.5
1	A	292	GLY	5.4
1	A	235	PHE	5.4
1	B	127	GLY	4.9
1	D	225	PRO	4.9
1	D	224	VAL	4.7
1	D	233	PRO	4.7
1	B	234	GLY	4.3
1	B	235	PHE	4.3
1	B	225	PRO	4.3
1	C	136	LEU	4.0
1	A	234	GLY	4.0
1	C	224	VAL	3.8
1	C	64	ALA	3.7
1	C	135	CYS	3.7
1	A	274	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	225	PRO	3.6
1	A	278	ALA	3.6
1	B	292	GLY	3.6
1	D	235	PHE	3.5
1	D	125	PRO	3.3
1	B	224	VAL	3.3
1	A	128	ASP	3.2
1	A	126	ALA	3.1
1	C	63	VAL	3.1
1	C	139	SER	3.0
1	B	38	ARG	3.0
1	D	128	ASP	3.0
1	A	276	GLY	3.0
1	B	233	PRO	3.0
1	C	140	PHE	2.9
1	C	223	GLN	2.7
1	D	126	ALA	2.7
1	C	137	GLY	2.7
1	D	136	LEU	2.6
1	D	274	ARG	2.6
1	A	197	ASP	2.6
1	C	65	CYS	2.5
1	B	124	VAL	2.5
1	B	140	PHE	2.5
1	A	201	ASP	2.4
1	C	172	ILE	2.4
1	C	66	GLY	2.4
1	B	199	THR	2.4
1	C	134	ILE	2.4
1	A	222	VAL	2.3
1	A	223	GLN	2.3
1	C	138	ASN	2.3
1	B	121	ASP	2.3
1	A	198	LEU	2.3
1	C	235	PHE	2.2
1	D	135	CYS	2.2
1	C	91	LEU	2.2
1	A	199	THR	2.1
1	B	263	GLN	2.1
1	A	140	PHE	2.1
1	C	141	ALA	2.1
1	B	261	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLN	2.1
1	B	166	PRO	2.1
1	C	292	GLY	2.1
1	D	64	ALA	2.1
1	D	66	GLY	2.0
1	C	142	HIS	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	TAM	A	1500	11/11	0.82	0.34	6.01	33,41,44,44	0
2	C2F	D	1200	33/33	0.78	0.24	5.28	48,53,61,65	0
3	TAM	D	1400	11/11	0.73	0.37	4.94	27,37,41,42	0
2	C2F	A	1100	33/33	0.79	0.22	3.64	40,49,65,66	0
3	TAM	C	1600	11/11	0.82	0.36	2.94	14,20,35,36	0
2	C2F	B	1700	33/33	0.75	0.21	2.78	47,72,77,78	0
2	C2F	C	1410	33/33	0.82	0.20	1.74	19,29,55,57	0

6.5 Other polymers (i)

There are no such residues in this entry.