Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:51 PM GMT

PDB ID	:	1MC3
Title	:	CRYSTAL STRUCTURE OF RFFH
Authors	:	Sivaraman, J.; Sauve, V.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2002-08-05
Resolution	:	2.60 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 ⓘ symbol.

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

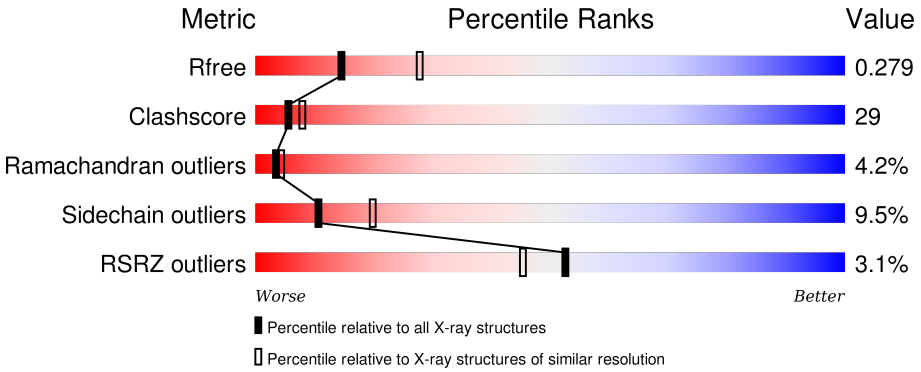
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	296	3% 53% 38% 6%
1	B	296	3% 60% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4557 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	Se	0	0	0
			2166	1390	359	410	2	5			
1	B	291	Total	C	N	O	S	Se	0	0	0
			2166	1390	359	410	2	5			

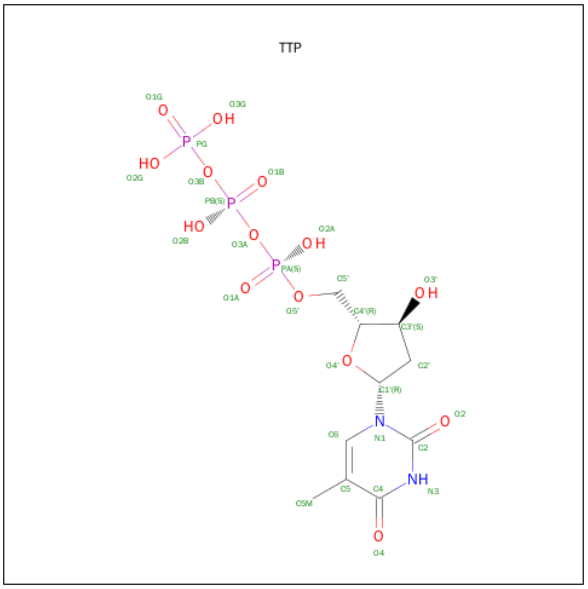
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P61887
A	-1	SER	-	CLONING ARTIFACT	UNP P61887
A	0	HIS	-	CLONING ARTIFACT	UNP P61887
A	1	MSE	MET	MODIFIED RESIDUE	UNP P61887
A	33	MSE	MET	MODIFIED RESIDUE	UNP P61887
A	42	MSE	MET	MODIFIED RESIDUE	UNP P61887
A	138	MSE	MET	MODIFIED RESIDUE	UNP P61887
A	203	MSE	MET	MODIFIED RESIDUE	UNP P61887
B	-2	GLY	-	CLONING ARTIFACT	UNP P61887
B	-1	SER	-	CLONING ARTIFACT	UNP P61887
B	0	HIS	-	CLONING ARTIFACT	UNP P61887
B	1	MSE	MET	MODIFIED RESIDUE	UNP P61887
B	33	MSE	MET	MODIFIED RESIDUE	UNP P61887
B	42	MSE	MET	MODIFIED RESIDUE	UNP P61887
B	138	MSE	MET	MODIFIED RESIDUE	UNP P61887
B	203	MSE	MET	MODIFIED RESIDUE	UNP P61887

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is water.

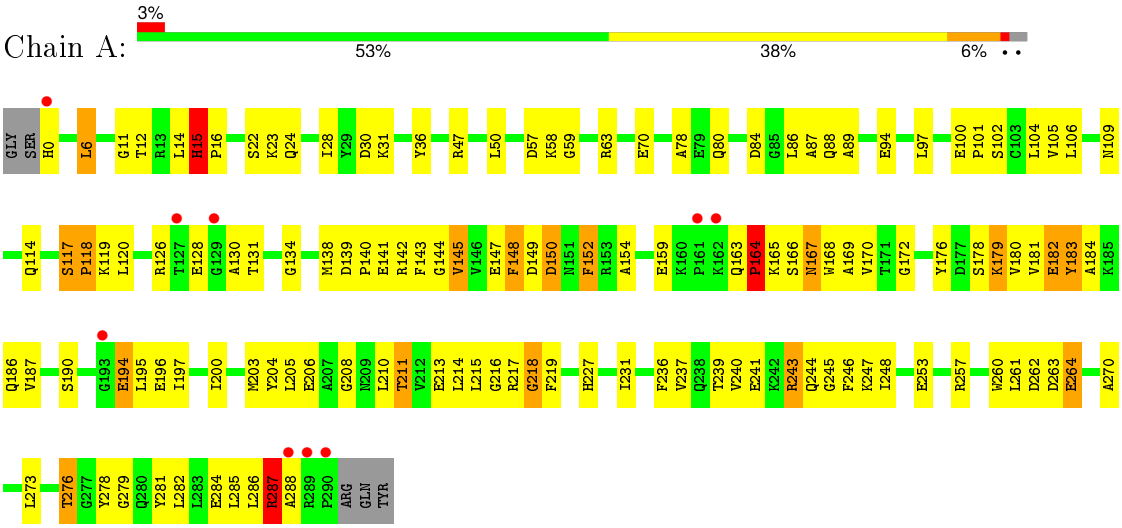
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	95	Total	O	0	0
			95	95		

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.

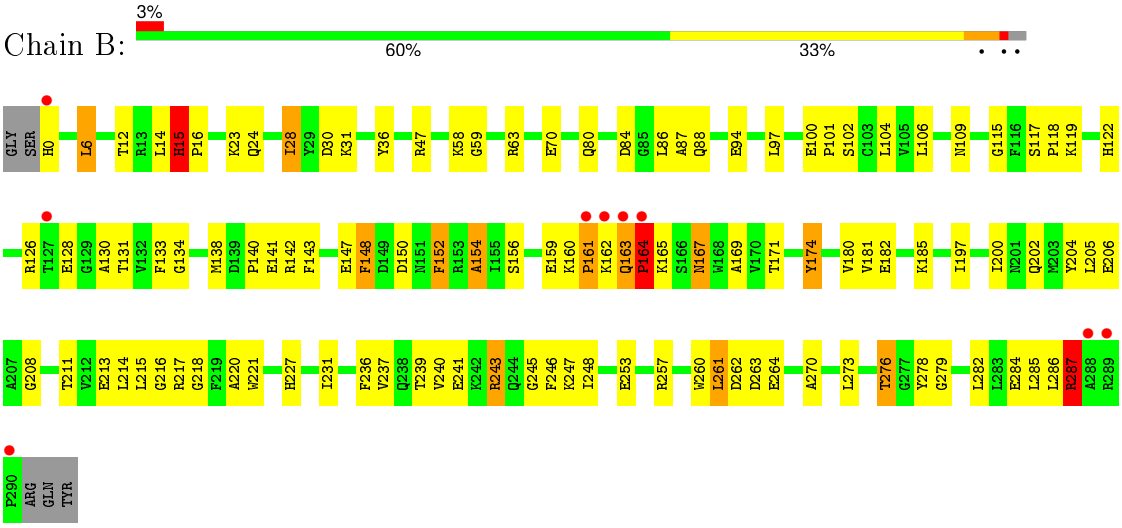
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.34Å 71.68Å 59.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.4 (20.00-2.60) 84.5 (19.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.280 0.223 , 0.279	Depositor DCC
R_{free} test set	1661 reflections (10.05%)	DCC
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.3	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 16531 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4557	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: MG, TTP

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	0.59	0/2211	0.79	3/2991 (0.1%)
1	B	0.58	0/2211	0.81	4/2991 (0.1%)
All	All	0.58	0/4422	0.80	7/5982 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	HIS	N-CA-C	7.96	132.49	111.00
1	B	15	HIS	N-CA-C	7.76	131.95	111.00
1	A	15	HIS	C-N-CD	6.35	141.74	128.40
1	B	15	HIS	C-N-CD	6.01	141.03	128.40
1	B	28	ILE	N-CA-C	-5.38	96.47	111.00
1	B	245	GLY	N-CA-C	5.14	125.95	113.10
1	A	245	GLY	N-CA-C	5.00	125.61	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	2166	0	2042	137	0
1	B	2166	0	2042	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	1	0
3	B	29	0	13	0	0
4	A	70	0	0	10	0
4	B	95	0	0	12	0
All	All	4557	0	4110	250	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 29.

All (250) 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:80:GLN:HE21	1:A:88:GLN:HE21	1.00	0.98
1:B:126:ARG:NH1	1:B:211:THR:HG21	1.80	0.97
1:B:80:GLN:HE21	1:B:88:GLN:HE21	0.97	0.93
1:A:119:LYS:HE3	1:A:213:GLU:HG3	1.56	0.87
1:B:276:THR:HG23	1:B:278:TYR:H	1.41	0.85
1:B:276:THR:HG22	1:B:279:GLY:H	1.41	0.84
1:A:276:THR:HG23	1:A:278:TYR:H	1.43	0.82
1:A:276:THR:HG22	1:A:279:GLY:H	1.45	0.82
1:B:80:GLN:HE21	1:B:88:GLN:NE2	1.80	0.79
1:B:117:SER:OG	1:B:118:PRO:HD3	1.83	0.79
1:A:257:ARG:HH11	1:A:257:ARG:CB	1.96	0.79
1:B:94:GLU:HG3	1:B:181:VAL:HG11	1.65	0.78
1:B:141:GLU:O	1:B:160:LYS:HA	1.85	0.76
1:B:257:ARG:CB	1:B:257:ARG:HH11	1.99	0.76
1:B:122:HIS:HB2	4:B:462:HOH:O	1.85	0.76
1:A:257:ARG:NH1	1:A:257:ARG:HB2	2.00	0.75
1:B:80:GLN:NE2	1:B:88:GLN:HE21	1.80	0.74
1:B:6:LEU:HD22	1:B:104:LEU:HD11	1.67	0.74
1:A:15:HIS:O	1:A:16:PRO:C	2.21	0.74
1:B:126:ARG:HH11	1:B:211:THR:HG21	1.50	0.74
1:A:6:LEU:HD22	1:A:104:LEU:HD11	1.69	0.74
1:A:114:GLN:HA	1:A:114:GLN:NE2	2.04	0.73
1:A:80:GLN:NE2	1:A:88:GLN:HE21	1.82	0.72
1:A:94:GLU:HG3	1:A:181:VAL:HG11	1.71	0.72
1:B:15:HIS:O	1:B:16:PRO:C	2.21	0.72
1:B:257:ARG:HB2	1:B:257:ARG:NH1	2.04	0.72
1:A:257:ARG:HH11	1:A:257:ARG:HB3	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH1	1:A:257:ARG:CB	2.53	0.71
1:A:152:PHE:O	1:A:154:ALA:N	2.23	0.70
1:B:161:PRO:O	1:B:163:GLN:N	2.24	0.70
1:B:130:ALA:O	1:B:211:THR:HG22	1.92	0.70
1:B:257:ARG:HB3	1:B:257:ARG:HH11	1.55	0.70
1:A:100:GLU:HB3	1:A:101:PRO:HD2	1.73	0.70
1:B:148:PHE:N	1:B:148:PHE:CD1	2.59	0.70
1:A:138:MSE:C	1:A:140:PRO:HD3	2.12	0.70
1:B:163:GLN:CB	1:B:164:PRO:HD3	2.22	0.69
1:A:236:PHE:CD1	1:B:243:ARG:HG2	2.27	0.69
1:A:126:ARG:NH1	1:A:211:THR:HG21	2.06	0.69
1:B:148:PHE:N	1:B:148:PHE:HD1	1.91	0.69
1:B:217:ARG:HG3	1:B:218:GLY:N	2.08	0.69
1:B:31:LYS:HE2	1:B:248:ILE:O	1.93	0.69
1:B:257:ARG:HD3	4:B:376:HOH:O	1.93	0.69
1:B:257:ARG:NH1	1:B:257:ARG:CB	2.56	0.69
1:A:178:SER:O	1:A:180:VAL:N	2.26	0.68
1:B:239:THR:O	1:B:243:ARG:HB2	1.93	0.68
1:B:237:VAL:O	1:B:241:GLU:HG3	1.94	0.67
1:A:243:ARG:HG2	1:B:236:PHE:CD1	2.29	0.67
1:B:148:PHE:HB2	1:B:152:PHE:O	1.95	0.66
1:B:167:ASN:HD22	1:B:167:ASN:H	1.44	0.66
1:A:147:GLU:HG2	1:A:148:PHE:H	1.61	0.66
1:A:190:SER:HB3	1:A:196:GLU:HG3	1.78	0.66
1:A:186:GLN:O	1:A:186:GLN:HG3	1.96	0.66
1:B:276:THR:CG2	1:B:278:TYR:HB3	2.26	0.65
1:A:239:THR:O	1:A:243:ARG:HB2	1.96	0.65
1:A:152:PHE:C	1:A:154:ALA:H	2.00	0.65
1:A:31:LYS:HE2	1:A:248:ILE:O	1.96	0.65
1:B:270:ALA:HB2	1:B:282:LEU:HB3	1.78	0.65
1:A:253:GLU:HG3	1:A:285:LEU:CD1	2.27	0.65
1:A:28:ILE:HB	1:A:36:TYR:CE1	2.33	0.64
1:A:87:ALA:HB1	1:A:200:ILE:HD11	1.79	0.64
1:B:253:GLU:HG3	1:B:285:LEU:CD1	2.28	0.63
1:A:141:GLU:N	1:A:141:GLU:OE1	2.31	0.63
1:A:138:MSE:HB3	4:A:315:HOH:O	1.98	0.63
1:B:161:PRO:C	1:B:163:GLN:H	2.03	0.62
1:B:131:THR:HG23	1:B:211:THR:HG23	1.80	0.62
1:A:276:THR:CG2	1:A:278:TYR:HB3	2.30	0.61
1:B:115:GLY:O	1:B:118:PRO:HD2	1.99	0.61
1:B:100:GLU:HB3	1:B:101:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:H	1:A:167:ASN:HD22	1.49	0.61
1:B:181:VAL:HG12	4:B:303:HOH:O	2.00	0.60
1:A:194:GLU:O	1:A:196:GLU:HG2	2.01	0.60
1:A:154:ALA:O	1:A:205:LEU:HD11	2.02	0.60
1:A:270:ALA:HB2	1:A:282:LEU:HB3	1.84	0.60
1:B:159:GLU:HB2	4:B:464:HOH:O	2.02	0.59
1:A:237:VAL:O	1:A:241:GLU:HG3	2.03	0.59
1:A:205:LEU:HD13	1:A:210:LEU:HD23	1.85	0.59
1:B:28:ILE:HB	1:B:36:TYR:CE1	2.38	0.58
1:B:30:ASP:OD2	1:B:247:LYS:HE3	2.03	0.58
1:A:205:LEU:HD12	4:A:323:HOH:O	2.03	0.58
1:B:126:ARG:NH1	1:B:211:THR:CG2	2.64	0.58
1:B:119:LYS:HE2	4:B:364:HOH:O	2.04	0.58
1:A:80:GLN:HE21	1:A:88:GLN:NE2	1.85	0.57
1:A:206:GLU:C	1:A:208:GLY:N	2.56	0.57
1:B:152:PHE:O	1:B:154:ALA:N	2.34	0.57
1:B:197:ILE:HD12	1:B:200:ILE:HD12	1.86	0.57
1:B:276:THR:HG22	1:B:279:GLY:N	2.17	0.56
1:A:286:LEU:C	1:A:287:ARG:HD2	2.25	0.56
1:A:138:MSE:HE2	4:B:442:HOH:O	2.04	0.56
1:B:217:ARG:HG3	1:B:218:GLY:H	1.69	0.56
1:A:217:ARG:O	1:A:219:PHE:N	2.39	0.56
1:B:276:THR:HG21	1:B:278:TYR:HB3	1.88	0.55
1:A:217:ARG:CG	1:A:218:GLY:H	2.20	0.55
1:A:206:GLU:C	1:A:208:GLY:H	2.10	0.55
1:B:6:LEU:CD2	1:B:104:LEU:HD11	2.35	0.55
1:B:181:VAL:CG1	4:B:303:HOH:O	2.55	0.55
1:B:185:LYS:NZ	4:B:303:HOH:O	2.40	0.54
1:A:6:LEU:CD2	1:A:104:LEU:HD11	2.35	0.54
4:A:321:HOH:O	1:B:138:MSE:HG3	2.06	0.54
1:A:47:ARG:HG2	1:A:260:TRP:CZ2	2.43	0.54
1:B:0:HIS:HA	4:B:345:HOH:O	2.07	0.54
1:A:86:LEU:HD13	1:A:106:LEU:HD21	1.90	0.54
1:B:126:ARG:HH12	1:B:211:THR:HG21	1.68	0.54
1:A:178:SER:C	1:A:180:VAL:H	2.11	0.54
1:A:244:GLN:O	1:B:217:ARG:O	2.25	0.54
1:A:164:PRO:HG2	4:A:403:HOH:O	2.07	0.54
1:A:30:ASP:OD2	1:A:247:LYS:HE3	2.07	0.54
1:A:117:SER:HA	1:A:120:LEU:HD12	1.89	0.53
1:B:47:ARG:HG2	1:B:260:TRP:CZ2	2.43	0.53
1:A:119:LYS:HE3	1:A:213:GLU:CG	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:VAL:HG13	1:B:181:VAL:N	2.24	0.53
1:B:276:THR:CG2	1:B:278:TYR:H	2.18	0.53
1:A:147:GLU:HG2	1:A:148:PHE:N	2.23	0.53
1:B:154:ALA:O	1:B:205:LEU:HD11	2.08	0.53
1:A:217:ARG:HG3	1:A:218:GLY:N	2.23	0.53
1:A:147:GLU:O	1:A:148:PHE:HB3	2.09	0.53
1:B:161:PRO:C	1:B:163:GLN:N	2.62	0.52
1:A:276:THR:CG2	1:A:278:TYR:H	2.18	0.52
1:A:152:PHE:C	1:A:154:ALA:N	2.63	0.52
1:A:241:GLU:CD	1:A:247:LYS:HD3	2.30	0.52
1:A:287:ARG:HD2	1:A:287:ARG:N	2.24	0.52
1:A:217:ARG:CG	1:A:218:GLY:N	2.72	0.52
1:B:148:PHE:HD2	1:B:152:PHE:CA	2.22	0.52
1:B:286:LEU:C	1:B:287:ARG:HD2	2.31	0.52
1:B:97:LEU:CD2	1:B:102:SER:HB3	2.40	0.51
1:A:134:GLY:HA2	1:A:169:ALA:O	2.10	0.51
1:B:97:LEU:HD21	1:B:102:SER:HB3	1.92	0.51
1:B:261:LEU:O	1:B:261:LEU:HD12	2.10	0.51
1:A:179:LYS:O	1:A:183:TYR:CD2	2.64	0.51
1:B:287:ARG:HD2	1:B:287:ARG:N	2.25	0.51
1:A:288:ALA:HB3	4:A:395:HOH:O	2.10	0.51
1:A:84:ASP:HB2	1:A:88:GLN:NE2	2.27	0.51
1:B:148:PHE:HD1	1:B:148:PHE:H	1.59	0.51
1:B:47:ARG:HD2	1:B:260:TRP:NE1	2.26	0.50
1:A:139:ASP:N	1:A:140:PRO:HD3	2.25	0.50
1:A:217:ARG:HG3	1:A:218:GLY:H	1.73	0.50
1:A:183:TYR:HD2	1:A:183:TYR:H	1.59	0.50
1:B:86:LEU:HD13	1:B:106:LEU:HD21	1.93	0.50
1:A:276:THR:HG21	1:A:278:TYR:HB3	1.93	0.50
1:A:131:THR:HG23	1:A:211:THR:CG2	2.41	0.50
1:A:131:THR:HG23	1:A:211:THR:HG23	1.93	0.50
1:B:130:ALA:HB2	1:B:204:TYR:CD2	2.47	0.50
1:B:241:GLU:CD	1:B:247:LYS:HD3	2.32	0.50
4:A:321:HOH:O	1:B:138:MSE:HE2	2.11	0.49
1:A:114:GLN:HA	1:A:114:GLN:HE21	1.73	0.49
1:B:133:PHE:CD2	1:B:213:GLU:HB3	2.47	0.49
1:A:183:TYR:CD1	1:A:203:MSE:HB2	2.48	0.49
1:B:262:ASP:OD2	1:B:264:GLU:HB2	2.13	0.49
1:A:84:ASP:HB2	1:A:88:GLN:HE22	1.76	0.48
1:B:159:GLU:O	1:B:160:LYS:C	2.51	0.48
1:A:206:GLU:O	1:A:208:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:SER:C	1:A:180:VAL:N	2.67	0.48
1:A:149:ASP:O	1:A:150:ASP:C	2.52	0.48
1:B:148:PHE:HB2	1:B:152:PHE:C	2.33	0.48
1:A:23:LYS:HE3	1:A:24:GLN:HE22	1.79	0.48
1:B:23:LYS:HE3	1:B:24:GLN:HE22	1.79	0.48
1:B:284:GLU:O	1:B:287:ARG:HD3	2.14	0.47
1:A:253:GLU:HG3	1:A:285:LEU:HD11	1.95	0.47
1:A:243:ARG:HA	1:A:243:ARG:NE	2.29	0.47
1:B:253:GLU:HG3	1:B:285:LEU:HD11	1.96	0.47
1:B:84:ASP:HB2	1:B:88:GLN:HE22	1.80	0.47
1:A:244:GLN:HG2	1:B:220:ALA:HB2	1.96	0.47
1:B:284:GLU:HA	1:B:287:ARG:HD3	1.97	0.47
1:B:287:ARG:HG3	1:B:287:ARG:NH1	2.30	0.47
1:B:84:ASP:HB2	1:B:88:GLN:NE2	2.29	0.47
1:A:241:GLU:OE1	1:A:247:LYS:HD3	2.14	0.47
1:A:22:SER:HB2	1:A:57:ASP:CG	2.36	0.47
1:A:138:MSE:HG3	4:B:442:HOH:O	2.16	0.46
1:B:270:ALA:HB2	1:B:282:LEU:CB	2.42	0.46
1:B:147:GLU:HB3	1:B:156:SER:OG	2.16	0.46
1:B:167:ASN:N	1:B:167:ASN:HD22	2.13	0.46
1:A:167:ASN:N	1:A:167:ASN:HD22	2.10	0.46
1:B:241:GLU:OE2	1:B:247:LYS:HD3	2.15	0.46
1:B:287:ARG:HH11	1:B:287:ARG:HG3	1.80	0.46
1:A:276:THR:HG22	1:A:279:GLY:N	2.21	0.46
1:A:145:VAL:HG11	1:A:166:SER:O	2.14	0.46
1:B:217:ARG:CG	1:B:218:GLY:N	2.77	0.46
1:B:14:LEU:HA	1:B:227:HIS:CE1	2.51	0.46
1:A:241:GLU:OE2	1:A:247:LYS:HD3	2.15	0.46
1:B:206:GLU:C	1:B:208:GLY:H	2.18	0.46
1:A:119:LYS:HE2	1:A:215:LEU:HD23	1.98	0.45
1:A:100:GLU:CB	1:A:101:PRO:HD2	2.46	0.45
1:A:143:PHE:CB	4:A:314:HOH:O	2.63	0.45
1:A:183:TYR:HD1	1:A:203:MSE:HB2	1.81	0.45
1:A:97:LEU:HD21	1:A:102:SER:HB3	1.97	0.45
1:A:184:ALA:O	1:A:187:VAL:HG23	2.17	0.45
1:B:174:TYR:CD1	1:B:174:TYR:N	2.85	0.45
1:A:147:GLU:C	1:A:148:PHE:CD1	2.90	0.44
1:B:133:PHE:HA	1:B:213:GLU:O	2.16	0.44
1:B:134:GLY:HA2	1:B:169:ALA:O	2.18	0.44
1:A:164:PRO:HG2	1:A:165:LYS:H	1.82	0.44
1:B:126:ARG:HH12	1:B:211:THR:CG2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:OH	1:B:217:ARG:NH2	2.51	0.44
1:A:243:ARG:HG2	1:B:236:PHE:CG	2.51	0.44
1:A:147:GLU:C	1:A:148:PHE:HD1	2.21	0.44
1:A:50:LEU:HD11	1:A:78:ALA:CB	2.48	0.44
1:B:273:LEU:O	1:B:276:THR:HB	2.18	0.43
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.87	0.43
1:B:276:THR:HG23	1:B:278:TYR:N	2.20	0.43
1:A:118:PRO:O	1:A:119:LYS:C	2.56	0.43
1:A:131:THR:HA	1:A:211:THR:HG22	1.99	0.43
1:A:240:VAL:HG21	1:A:248:ILE:HD11	2.01	0.43
1:A:284:GLU:O	1:A:287:ARG:HD3	2.19	0.43
1:A:287:ARG:NH1	1:A:287:ARG:HG3	2.34	0.43
1:A:22:SER:HB2	1:A:57:ASP:OD2	2.18	0.43
1:A:6:LEU:HD21	1:A:89:ALA:HB2	2.01	0.43
1:B:87:ALA:HB1	1:B:200:ILE:HD11	2.01	0.43
1:B:206:GLU:C	1:B:208:GLY:N	2.72	0.43
1:A:0:HIS:HA	4:A:330:HOH:O	2.18	0.43
1:B:276:THR:CG2	1:B:278:TYR:N	2.81	0.43
1:B:12:THR:O	1:B:15:HIS:HB2	2.18	0.43
1:A:287:ARG:HH11	1:A:287:ARG:HG3	1.84	0.43
1:A:59:GLY:O	1:A:63:ARG:HB2	2.19	0.43
1:A:138:MSE:CB	4:A:315:HOH:O	2.61	0.42
1:B:243:ARG:NE	1:B:243:ARG:HA	2.34	0.42
1:A:183:TYR:N	1:A:183:TYR:CD2	2.88	0.42
1:A:273:LEU:O	1:A:276:THR:HB	2.19	0.42
1:B:134:GLY:O	1:B:215:LEU:HB2	2.18	0.42
1:A:168:TRP:CH2	1:A:214:LEU:HD21	2.55	0.42
1:A:12:THR:O	1:A:15:HIS:HB2	2.19	0.42
1:A:144:GLY:O	1:A:169:ALA:HA	2.19	0.42
1:B:171:THR:HG22	1:B:221:TRP:CE2	2.54	0.42
1:A:197:ILE:O	1:A:197:ILE:HG13	2.20	0.42
1:A:284:GLU:HA	1:A:287:ARG:HD3	2.01	0.42
1:B:163:GLN:CB	1:B:164:PRO:CD	2.96	0.42
1:B:180:VAL:CG1	1:B:181:VAL:N	2.83	0.42
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.92	0.41
1:A:164:PRO:CG	1:A:165:LYS:H	2.33	0.41
1:A:170:VAL:HG13	4:A:396:HOH:O	2.19	0.41
1:A:195:LEU:HD23	1:A:195:LEU:N	2.35	0.41
1:A:117:SER:O	1:A:120:LEU:HB2	2.19	0.41
1:B:143:PHE:CB	4:B:339:HOH:O	2.68	0.41
1:B:140:PRO:O	1:B:141:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:O	1:A:210:LEU:HG	2.21	0.41
1:B:264:GLU:HG2	4:B:432:HOH:O	2.19	0.41
1:A:130:ALA:HB2	1:A:204:TYR:CD2	2.55	0.41
1:B:59:GLY:O	1:B:63:ARG:HB2	2.20	0.41
1:A:257:ARG:CZ	1:A:257:ARG:HB2	2.50	0.41
1:A:179:LYS:O	1:A:182:GLU:HB2	2.21	0.41
1:A:97:LEU:CD2	1:A:102:SER:HB3	2.50	0.41
1:A:183:TYR:HD2	1:A:183:TYR:N	2.19	0.41
1:A:176:TYR:OH	1:A:197:ILE:HD11	2.21	0.41
1:A:11:GLY:HA2	3:A:294:TTP:O3B	2.21	0.41
1:B:240:VAL:HG21	1:B:248:ILE:HD11	2.03	0.41
1:B:47:ARG:CG	1:B:260:TRP:CZ2	3.03	0.41
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.95	0.40
1:A:105:VAL:HA	1:A:172:GLY:O	2.22	0.40
1:B:115:GLY:C	1:B:118:PRO:HD2	2.42	0.40
1:A:14:LEU:HA	1:A:227:HIS:CE1	2.56	0.40
1:A:262:ASP:OD2	1:A:264:GLU:HB2	2.22	0.40
1:B:148:PHE:CE2	1:B:214:LEU:HD21	2.57	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	289/296 (98%)	243 (84%)	34 (12%)	12 (4%)	3 4
1	B	289/296 (98%)	246 (85%)	31 (11%)	12 (4%)	3 4
All	All	578/592 (98%)	489 (85%)	65 (11%)	24 (4%)	3 4

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	164	PRO
1	B	128	GLU
1	B	150	ASP
1	B	152	PHE
1	B	162	LYS
1	B	164	PRO
1	A	150	ASP
1	A	179	LYS
1	A	218	GLY
1	B	163	GLN
1	B	165	LYS
1	A	128	GLU
1	A	142	ARG
1	A	152	PHE
1	B	142	ARG
1	B	161	PRO
1	A	287	ARG
1	B	154	ALA
1	A	148	PHE
1	B	287	ARG
1	A	216	GLY
1	A	118	PRO
1	B	216	GLY

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	211/240 (88%)	189 (90%)	22 (10%)	9 16
1	B	211/240 (88%)	193 (92%)	18 (8%)	13 25
All	All	422/480 (88%)	382 (90%)	40 (10%)	11 20

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

Mol	Chain	Res	Type
1	A	6	LEU
1	A	15	HIS
1	A	58	LYS
1	A	70	GLU
1	A	109	ASN
1	A	117	SER
1	A	145	VAL
1	A	159	GLU
1	A	164	PRO
1	A	167	ASN
1	A	182	GLU
1	A	183	TYR
1	A	194	GLU
1	A	211	THR
1	A	231	ILE
1	A	243	ARG
1	A	246	PHE
1	A	261	LEU
1	A	263	ASP
1	A	264	GLU
1	A	276	THR
1	A	287	ARG
1	B	6	LEU
1	B	15	HIS
1	B	58	LYS
1	B	70	GLU
1	B	109	ASN
1	B	148	PHE
1	B	164	PRO
1	B	167	ASN
1	B	174	TYR
1	B	182	GLU
1	B	202	GLN
1	B	231	ILE
1	B	243	ARG
1	B	246	PHE
1	B	261	LEU
1	B	263	ASP
1	B	276	THR
1	B	287	ARG

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	24	GLN
1	A	88	GLN
1	A	114	GLN
1	A	136	GLN
1	A	167	ASN
1	A	186	GLN
1	B	24	GLN
1	B	88	GLN
1	B	114	GLN
1	B	136	GLN
1	B	167	ASN
1	B	227	HIS

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
3	TTP	A	294	2	21,30,30	2.01	4 (19%)	31,47,47	1.95	6 (19%)
3	TTP	B	295	2	21,30,30	2.08	8 (38%)	31,47,47	1.98	7 (22%)

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
3	TTP	A	294	2	-	0/18/34/34	0/2/2/2
3	TTP	B	295	2	-	0/18/34/34	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	294	TTP	C3'-C4'	-4.76	1.39	1.53
3	B	295	TTP	C3'-C4'	-4.69	1.39	1.53
3	A	294	TTP	C2'-C1'	-4.49	1.39	1.52
3	B	295	TTP	C2'-C1'	-4.45	1.39	1.52
3	A	294	TTP	C2'-C3'	-3.86	1.42	1.52
3	B	295	TTP	C2'-C3'	-3.56	1.43	1.52
3	B	295	TTP	PG-O2G	-2.36	1.46	1.54
3	B	295	TTP	PG-O3G	-2.18	1.46	1.54
3	B	295	TTP	PA-O2A	-2.04	1.46	1.54
3	B	295	TTP	C5'-C4'	-2.03	1.45	1.51
3	B	295	TTP	C4-N3	2.61	1.37	1.33
3	A	294	TTP	C4-N3	2.76	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	294	TTP	C5-C4-N3	-5.72	118.77	125.14
3	B	295	TTP	C5-C4-N3	-5.60	118.91	125.14
3	B	295	TTP	PB-O3A-PA	-2.96	124.42	132.73
3	A	294	TTP	PB-O3A-PA	-2.63	125.34	132.73
3	A	294	TTP	O4'-C1'-C2'	-2.51	101.27	106.27
3	B	295	TTP	O4'-C1'-C2'	-2.02	102.24	106.27
3	B	295	TTP	O3A-PA-O5'	2.03	108.32	102.94
3	B	295	TTP	O2B-PB-O1B	2.40	125.56	112.53
3	A	294	TTP	O2B-PB-O1B	2.41	125.58	112.53
3	A	294	TTP	C2'-C3'-C4'	2.87	108.72	102.77
3	B	295	TTP	C2'-C3'-C4'	2.88	108.73	102.77
3	A	294	TTP	C4-N3-C2	5.46	119.97	115.25
3	B	295	TTP	C4-N3-C2	5.56	120.06	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	294	TTP	1	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	286/296 (96%)	-0.01	9 (3%) 52 45	34, 49, 60, 68	0
1	B	286/296 (96%)	0.04	9 (3%) 52 45	34, 48, 60, 68	0
All	All	572/592 (96%)	0.01	18 (3%) 52 45	34, 48, 60, 68	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	PRO	9.3
1	B	290	PRO	9.3
1	B	289	ARG	7.7
1	B	288	ALA	5.0
1	A	288	ALA	4.7
1	A	289	ARG	4.2
1	B	163	GLN	4.0
1	A	127	THR	3.8
1	B	162	LYS	3.8
1	A	193	GLY	3.4
1	A	0	HIS	3.1
1	B	161	PRO	3.1
1	A	162	LYS	3.0
1	A	161	PRO	2.5
1	B	0	HIS	2.3
1	A	129	GLY	2.3
1	B	127	THR	2.1
1	B	164	PRO	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 (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	TTP	B	295	29/29	0.98	0.11	-1.23	32,38,43,43	0
3	TTP	A	294	29/29	0.97	0.09	-2.13	33,38,43,43	0
2	MG	A	301	1/1	0.74	0.19	-	39,39,39,39	0
2	MG	B	302	1/1	0.95	0.04	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.