



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:35 AM GMT

PDB ID : 2UXH  
Title : TTGR IN COMPLEX WITH QUERCETIN  
Authors : Alguel, Y.; Meng, C.; Teran, W.; Krell, T.; Ramos, J.L.; Gallegos, M.-T.; Zhang, X.  
Deposited on : 2007-03-28  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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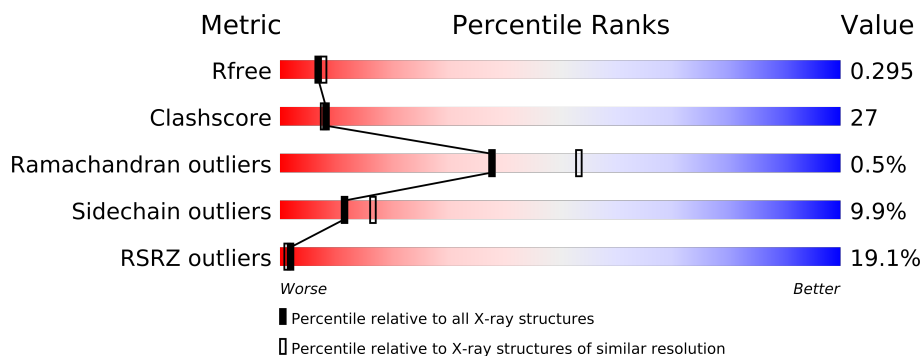
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	210	
1	B	210	

## 2 Entry composition i

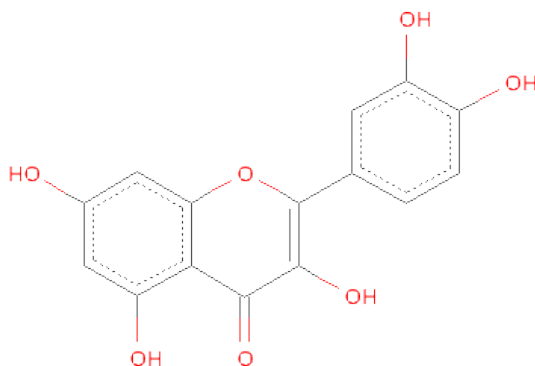
There are 3 unique types of molecules in this entry. The entry contains 3435 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1601	1001	293	299	8			
1	B	205	Total	C	N	O	S	0	0	0
			1599	997	296	298	8			

- Molecule 2 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	15	7		
2	B	1	Total	C	O	0	0
			22	15	7		

- Molecule 3 is water.

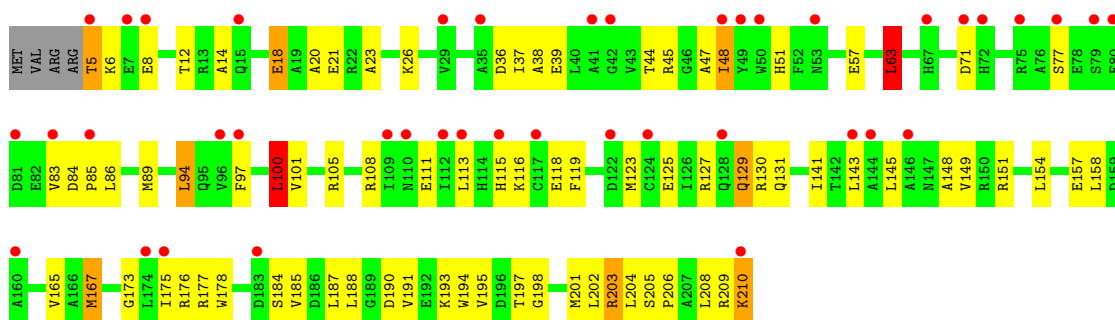
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 107	O 107	0	0
3	B	84	Total 84	O 84	0	0

### 3 Residue-property plots

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.

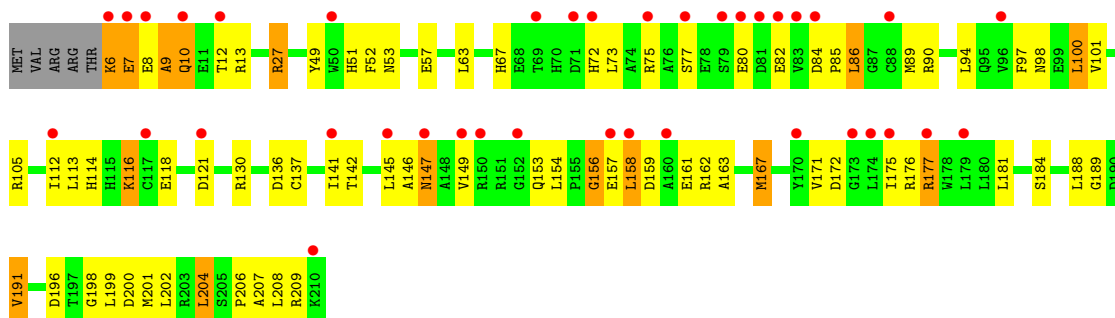
#### • Molecule 1: HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR

Chain A: 



#### • Molecule 1: HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.65Å 231.88Å 44.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 2.40 43.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	84.8 (44.32-2.40) 84.8 (43.28-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.237 , 0.295 0.232 , 0.295	Depositor DCC
$R_{free}$ test set	1273 reflections (8.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.7	EDS
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16721 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUE

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	0.55	0/1625	0.81	5/2199 (0.2%)
1	B	0.57	0/1623	0.75	2/2197 (0.1%)
All	All	0.56	0/3248	0.78	7/4396 (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	B	0	3
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	THR	CA-C-N	-9.80	95.64	117.20
1	A	5	THR	O-C-N	8.55	136.38	122.70
1	A	100	LEU	CA-CB-CG	6.61	130.50	115.30
1	A	45	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	156	GLY	N-CA-C	5.29	126.31	113.10
1	B	158	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	63	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	THR	Mainchain
1	B	6	LYS	Peptide
1	B	7	GLU	Peptide
1	B	9	ALA	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1601	0	1578	95	0
1	B	1599	0	1574	81	0
2	A	22	0	6	8	0
2	B	22	0	7	2	0
3	A	107	0	0	53	0
3	B	84	0	0	33	0
All	All	3435	0	3165	170	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (170) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:VAL:HG22	3:A:2084:HOH:O	1.43	1.18
1:A:176:ARG:HD3	1:B:176:ARG:NH1	1.56	1.18
1:A:39:GLU:HG2	3:A:2022:HOH:O	1.45	1.15
1:A:18:GLU:OE2	1:A:18:GLU:HA	1.40	1.13
1:A:23:ALA:HB3	3:A:2011:HOH:O	1.49	1.11
3:A:2099:HOH:O	1:B:204:LEU:HD12	1.53	1.08
1:A:143:LEU:HB3	3:A:2043:HOH:O	1.53	1.06
1:A:185:VAL:HG11	3:A:2079:HOH:O	1.56	1.04
1:A:204:LEU:HG	3:A:2097:HOH:O	1.60	1.01
1:A:154:LEU:HB2	3:A:2070:HOH:O	1.63	0.99
1:A:167:MET:HG2	3:A:2105:HOH:O	1.62	0.97
1:A:100:LEU:HG	3:A:2055:HOH:O	1.66	0.93
1:B:112:ILE:HG23	3:B:2011:HOH:O	1.69	0.91
1:A:100:LEU:HD23	3:A:2052:HOH:O	1.68	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:159:ASP:HB3	3:B:2063:HOH:O	1.73	0.89
1:B:73:LEU:HB2	3:B:2027:HOH:O	1.73	0.89
1:B:9:ALA:HB3	1:B:12:THR:OG1	1.71	0.88
1:B:7:GLU:N	1:B:8:GLU:O	2.06	0.87
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.38	0.87
1:A:18:GLU:OE1	1:A:105:ARG:HD2	1.75	0.87
1:A:209:ARG:HG2	3:A:2074:HOH:O	1.74	0.86
1:B:196:ASP:HA	3:B:2074:HOH:O	1.74	0.85
1:B:158:LEU:HA	3:B:2057:HOH:O	1.76	0.85
1:A:20:ALA:HA	3:A:2011:HOH:O	1.76	0.85
1:A:205:SER:HA	3:A:2099:HOH:O	1.77	0.85
2:A:1211:QUE:O27	2:A:1211:QUE:H19	1.78	0.83
1:B:184:SER:HB2	3:B:2066:HOH:O	1.77	0.82
1:A:38:ALA:HB2	1:A:48:ILE:HD11	1.64	0.80
1:B:82:GLU:HG2	3:B:2031:HOH:O	1.81	0.79
2:A:1211:QUE:H16	3:A:2078:HOH:O	1.82	0.79
1:A:184:SER:HB3	3:A:2090:HOH:O	1.84	0.78
1:B:199:LEU:HB2	3:B:2074:HOH:O	1.82	0.77
1:A:37:ILE:HG12	3:A:2011:HOH:O	1.83	0.77
1:A:36:ASP:HB2	3:A:2019:HOH:O	1.85	0.77
1:A:202:LEU:HD23	3:A:2096:HOH:O	1.84	0.77
1:A:194:TRP:HA	3:A:2077:HOH:O	1.85	0.76
1:A:111:GLU:OE1	1:A:115:HIS:HD2	1.67	0.76
1:B:159:ASP:HB2	3:B:2082:HOH:O	1.88	0.73
1:A:47:ALA:O	1:A:51:HIS:HD2	1.71	0.73
3:A:2099:HOH:O	1:B:200:ASP:HB3	1.89	0.72
1:B:199:LEU:HD12	3:B:2074:HOH:O	1.89	0.71
1:B:77:SER:HB2	3:B:2037:HOH:O	1.90	0.71
1:A:18:GLU:OE2	1:A:18:GLU:CA	2.30	0.70
1:A:206:PRO:HD3	3:A:2099:HOH:O	1.92	0.69
1:A:176:ARG:CD	1:B:176:ARG:NH1	2.48	0.69
1:B:77:SER:CB	3:B:2037:HOH:O	2.41	0.69
1:B:163:ALA:HB1	1:B:202:LEU:HD22	1.75	0.69
1:B:159:ASP:CB	3:B:2063:HOH:O	2.35	0.69
1:B:27:ARG:NH1	1:B:27:ARG:HG2	2.04	0.69
1:A:209:ARG:O	1:A:210:LYS:HB2	1.92	0.68
1:A:176:ARG:HD3	1:B:176:ARG:CZ	2.22	0.68
1:A:176:ARG:NH1	3:A:2080:HOH:O	2.27	0.68
2:A:1211:QUE:O27	2:A:1211:QUE:C19	2.41	0.66
1:A:84:ASP:HB3	3:A:2046:HOH:O	1.96	0.66
1:A:203:ARG:HG3	3:A:2097:HOH:O	1.95	0.65
1:A:157:GLU:HG3	3:A:2074:HOH:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:PHE:O	1:A:101:VAL:HG23	1.97	0.64
1:A:176:ARG:NH1	1:B:176:ARG:HD2	2.14	0.63
1:B:116:LYS:HB3	3:B:2011:HOH:O	1.99	0.62
1:B:142:THR:HB	3:B:2055:HOH:O	1.98	0.62
3:A:2099:HOH:O	1:B:204:LEU:CD1	2.28	0.62
2:B:1211:QUE:O27	2:B:1211:QUE:H19	1.99	0.62
1:A:38:ALA:HB2	1:A:48:ILE:CD1	2.30	0.61
1:B:201:MET:HA	3:B:2078:HOH:O	2.00	0.61
1:A:167:MET:HB2	1:A:202:LEU:HD21	1.81	0.61
1:A:197:THR:HB	3:A:2077:HOH:O	2.00	0.61
1:B:67:HIS:HE1	3:B:2022:HOH:O	1.82	0.61
1:B:206:PRO:HA	1:B:209:ARG:HD2	1.85	0.59
1:B:77:SER:HA	3:B:2031:HOH:O	2.02	0.59
1:A:176:ARG:HD3	1:B:176:ARG:HH12	1.61	0.58
1:B:86:LEU:HD21	1:B:199:LEU:HD22	1.85	0.58
1:A:47:ALA:O	1:A:51:HIS:CD2	2.56	0.57
1:A:71:ASP:HB3	3:A:2039:HOH:O	2.05	0.57
1:A:167:MET:CG	2:A:1211:QUE:O29	2.52	0.57
1:B:172:ASP:OD2	1:B:176:ARG:NH1	2.38	0.57
3:A:2080:HOH:O	1:B:176:ARG:HD2	2.05	0.56
1:A:108:ARG:CD	3:A:2054:HOH:O	2.52	0.56
1:A:108:ARG:HD3	3:A:2054:HOH:O	2.06	0.56
1:A:158:LEU:N	3:A:2074:HOH:O	2.39	0.55
1:A:201:MET:HG2	3:A:2096:HOH:O	2.05	0.55
1:B:147:ASN:HB2	3:B:2056:HOH:O	2.06	0.55
1:B:85:PRO:HA	3:B:2031:HOH:O	2.07	0.55
1:B:89:MET:CA	3:B:2037:HOH:O	2.56	0.54
1:A:187:LEU:O	1:A:191:VAL:HB	2.08	0.53
1:B:89:MET:N	3:B:2037:HOH:O	2.42	0.53
1:B:177:ARG:NE	3:B:2065:HOH:O	2.40	0.53
1:A:119:PHE:CD1	1:A:127:ARG:HG3	2.44	0.53
1:B:100:LEU:HD11	1:B:175:ILE:HG23	1.91	0.53
1:A:145:LEU:O	1:A:149:VAL:HG23	2.09	0.52
1:A:197:THR:CB	3:A:2077:HOH:O	2.58	0.52
1:B:49:TYR:HA	1:B:52:PHE:O	2.10	0.52
1:A:167:MET:HE2	1:A:167:MET:HA	1.92	0.52
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.16	0.52
1:A:167:MET:HG2	2:A:1211:QUE:O29	2.10	0.52
1:A:158:LEU:HA	3:A:2074:HOH:O	2.09	0.51
1:A:157:GLU:C	3:A:2074:HOH:O	2.48	0.51
3:A:2013:HOH:O	1:B:121:ASP:HB2	2.10	0.51
1:B:101:VAL:HG11	1:B:188:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:ALA:C	3:A:2070:HOH:O	2.49	0.51
1:B:90:ARG:NH2	3:B:2038:HOH:O	2.43	0.51
1:A:178:TRP:HZ3	3:A:2052:HOH:O	1.94	0.51
1:A:94:LEU:HD13	1:A:195:VAL:HG21	1.94	0.50
1:A:14:ALA:HA	3:A:2009:HOH:O	2.12	0.50
1:A:123:MET:HE3	3:A:2056:HOH:O	2.11	0.49
1:A:206:PRO:HD2	1:B:200:ASP:OD2	2.13	0.49
1:B:162:ARG:NH2	1:B:207:ALA:O	2.39	0.49
1:B:114:HIS:ND1	1:B:176:ARG:HD3	2.28	0.48
1:A:118:GLU:HG3	1:B:118:GLU:HG3	1.94	0.48
1:B:85:PRO:HD2	1:B:153:GLN:OE1	2.13	0.48
1:B:154:LEU:CD2	3:B:2075:HOH:O	2.62	0.48
2:B:1211:QUE:O27	2:B:1211:QUE:C19	2.60	0.48
1:B:13:ARG:HB2	1:B:51:HIS:CE1	2.48	0.47
1:A:21:GLU:OE1	1:A:108:ARG:HD2	2.14	0.47
1:A:131:GLN:HB3	1:B:181:LEU:HD21	1.96	0.47
1:A:8:GLU:CG	3:A:2006:HOH:O	2.63	0.47
1:A:167:MET:HG3	2:A:1211:QUE:O29	2.15	0.46
1:A:149:VAL:N	3:A:2070:HOH:O	2.48	0.46
1:B:112:ILE:HA	1:B:116:LYS:HB3	1.97	0.46
1:B:6:LYS:N	1:B:10:GLN:HB3	2.30	0.46
1:A:63:LEU:O	1:A:63:LEU:HD12	2.15	0.46
1:B:154:LEU:HD21	3:B:2075:HOH:O	2.16	0.46
1:B:142:THR:HG21	1:B:161:GLU:HG2	1.98	0.45
1:B:198:GLY:O	1:B:201:MET:HB3	2.16	0.45
1:B:149:VAL:HG12	1:B:154:LEU:HB2	1.99	0.45
1:A:8:GLU:O	1:A:12:THR:HG23	2.16	0.45
1:A:115:HIS:HE1	3:A:2081:HOH:O	1.99	0.45
1:B:167:MET:HG3	1:B:202:LEU:HD21	2.00	0.44
1:A:119:PHE:CG	1:A:127:ARG:HG3	2.52	0.44
1:A:116:LYS:HA	1:B:118:GLU:HG2	1.98	0.44
1:A:8:GLU:HG2	3:A:2006:HOH:O	2.18	0.44
1:A:151:ARG:NH2	3:A:2072:HOH:O	2.50	0.44
1:B:189:GLY:H	1:B:191:VAL:HG22	1.84	0.43
1:A:48:ILE:H	1:A:48:ILE:HG13	1.52	0.43
1:B:82:GLU:HG3	1:B:84:ASP:H	1.83	0.43
1:A:116:LYS:C	1:B:118:GLU:HG2	2.38	0.43
1:A:190:ASP:O	1:A:193:LYS:N	2.51	0.43
1:A:167:MET:HE1	1:A:198:GLY:HA3	2.01	0.43
1:A:111:GLU:OE1	1:A:115:HIS:CD2	2.58	0.43
1:A:100:LEU:HD11	1:A:175:ILE:HG12	2.01	0.42
1:B:75:ARG:NH2	3:B:2030:HOH:O	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:53:ASN:ND2	1:B:57:GLU:OE2	2.52	0.42
1:B:85:PRO:HB3	3:B:2056:HOH:O	2.20	0.42
1:B:72:HIS:HD2	3:B:2029:HOH:O	2.02	0.42
1:B:137:CYS:O	1:B:141:ILE:HG13	2.20	0.42
1:A:84:ASP:N	1:A:85:PRO:HD3	2.34	0.42
1:A:151:ARG:HD3	3:A:2045:HOH:O	2.19	0.42
1:A:167:MET:HE1	1:A:198:GLY:CA	2.50	0.42
1:A:83:VAL:C	1:A:85:PRO:HD3	2.39	0.42
1:B:97:PHE:CZ	1:B:171:VAL:HG13	2.54	0.42
1:A:141:ILE:HG12	2:A:1211:QUE:C1	2.49	0.42
1:B:86:LEU:HD22	3:B:2036:HOH:O	2.19	0.42
1:A:125:GLU:O	1:A:129:GLN:HB2	2.19	0.42
1:A:158:LEU:CA	3:A:2074:HOH:O	2.67	0.42
1:B:85:PRO:CB	3:B:2056:HOH:O	2.67	0.42
1:A:165:VAL:HA	3:B:2065:HOH:O	2.20	0.41
1:A:14:ALA:CA	3:A:2009:HOH:O	2.66	0.41
1:B:177:ARG:CZ	3:B:2065:HOH:O	2.68	0.41
1:B:145:LEU:O	1:B:149:VAL:HG13	2.20	0.41
1:A:197:THR:HG23	1:B:208:LEU:HG	2.03	0.41
1:B:167:MET:HG3	1:B:202:LEU:HD11	2.01	0.41
1:A:101:VAL:HG11	1:A:188:LEU:HB2	2.02	0.41
1:A:8:GLU:HG3	3:A:2006:HOH:O	2.21	0.41
1:A:167:MET:HA	1:A:167:MET:CE	2.51	0.41
1:B:90:ARG:O	1:B:94:LEU:HG	2.21	0.41
2:A:1211:QUE:O30	3:A:2103:HOH:O	2.22	0.40
1:B:146:ALA:O	1:B:149:VAL:HG22	2.21	0.40
1:A:173:GLY:HA2	1:B:176:ARG:HH22	1.85	0.40
1:A:86:LEU:HD12	1:A:89:MET:HE2	2.02	0.40
1:A:208:LEU:CD1	3:A:2096:HOH:O	2.69	0.40
1:B:156:GLY:O	1:B:157:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	204/210 (97%)	191 (94%)	13 (6%)	0	100	100
1	B	203/210 (97%)	187 (92%)	14 (7%)	2 (1%)	22	32
All	All	407/420 (97%)	378 (93%)	27 (7%)	2 (0%)	38	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	B	204	LEU

### 5.3.2 Protein sidechains ⓘ

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	162/175 (93%)	145 (90%)	17 (10%)	10	14
1	B	162/175 (93%)	147 (91%)	15 (9%)	13	19
All	All	324/350 (93%)	292 (90%)	32 (10%)	11	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	18	GLU
1	A	26	LYS
1	A	44	THR
1	A	48	ILE
1	A	57	GLU
1	A	63	LEU
1	A	77	SER
1	A	94	LEU
1	A	100	LEU
1	A	113	LEU
1	A	129	GLN
1	A	130	ARG
1	A	167	MET
1	A	177	ARG

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Mol	Chain	Res	Type
1	A	203	ARG
1	A	210	LYS
1	B	27	ARG
1	B	63	LEU
1	B	80	GLU
1	B	86	LEU
1	B	98	ASN
1	B	100	LEU
1	B	105	ARG
1	B	113	LEU
1	B	116	LYS
1	B	130	ARG
1	B	136	ASP
1	B	147	ASN
1	B	167	MET
1	B	177	ARG
1	B	191	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	110	ASN
1	A	115	HIS
1	A	128	GLN
1	B	53	ASN
1	B	60	GLN
1	B	98	ASN
1	B	110	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	QUE	A	1211	-	23,24,24	1.50	2 (8%)	33,36,36	1.86	6 (18%)
2	QUE	B	1211	-	23,24,24	1.38	2 (8%)	33,36,36	1.42	6 (18%)

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	QUE	A	1211	-	-	0/4/4/4	0/1/3/3
2	QUE	B	1211	-	-	0/4/4/4	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1211	QUE	C14-C11	-5.01	1.39	1.46
2	B	1211	QUE	C14-C11	-4.07	1.41	1.46
2	B	1211	QUE	O12-C11	3.89	1.38	1.35
2	A	1211	QUE	O12-C11	3.79	1.38	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1211	QUE	O12-C11-C14	5.31	121.01	113.25
2	B	1211	QUE	O12-C11-C14	4.58	119.95	113.25
2	A	1211	QUE	C11-O12-C4	-4.30	116.53	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1211	QUE	C5-C4-C3	-3.87	118.37	123.10
2	B	1211	QUE	C5-C4-C3	-3.60	118.71	123.10
2	B	1211	QUE	O12-C4-C5	3.00	119.82	116.02
2	A	1211	QUE	C2-C3-C4	2.83	121.27	117.77
2	A	1211	QUE	O12-C4-C5	2.57	119.28	116.02
2	A	1211	QUE	C10-C9-C3	-2.47	118.70	121.41
2	B	1211	QUE	O12-C11-C10	-2.27	120.54	121.54
2	B	1211	QUE	C11-O12-C4	-2.25	118.78	121.27
2	B	1211	QUE	C2-C3-C4	2.19	120.48	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	206/210 (98%)	1.34	41 (19%) 2 1	35, 53, 66, 72	0
1	B	205/210 (97%)	1.23	38 (18%) 2 1	35, 47, 64, 68	0
All	All	411/420 (97%)	1.28	79 (19%) 2 1	35, 50, 66, 72	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	VAL	10.7
1	A	5	THR	9.1
1	B	8	GLU	6.9
1	A	81	ASP	6.5
1	B	50	TRP	5.7
1	A	210	LYS	5.6
1	B	79	SER	5.6
1	B	81	ASP	5.3
1	B	72	HIS	5.3
1	B	10	GLN	4.9
1	A	83	VAL	4.8
1	A	50	TRP	4.3
1	A	124	CYS	4.1
1	B	84	ASP	3.9
1	A	42	GLY	3.8
1	A	75	ARG	3.8
1	A	8	GLU	3.8
1	B	80	GLU	3.8
1	A	7	GLU	3.7
1	B	149	VAL	3.7
1	A	79	SER	3.7
1	B	7	GLU	3.6
1	B	152	GLY	3.4
1	B	147	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLU	3.4
1	A	77	SER	3.4
1	B	6	LYS	3.3
1	A	72	HIS	3.3
1	B	210	LYS	3.1
1	A	146	ALA	3.1
1	B	174	LEU	3.0
1	B	158	LEU	3.0
1	B	82	GLU	3.0
1	B	71	ASP	3.0
1	A	175	ILE	3.0
1	A	122	ASP	2.9
1	A	48	ILE	2.9
1	A	110	ASN	2.9
1	A	29	VAL	2.8
1	B	173	GLY	2.8
1	B	170	TYR	2.8
1	A	67	HIS	2.8
1	A	80	GLU	2.8
1	B	88	CYS	2.7
1	A	112	ILE	2.7
1	B	12	THR	2.7
1	A	174	LEU	2.6
1	B	175	ILE	2.6
1	A	97	PHE	2.6
1	A	53	ASN	2.6
1	A	85	PRO	2.6
1	B	69	THR	2.6
1	A	113	LEU	2.5
1	B	179	LEU	2.5
1	A	183	ASP	2.5
1	A	49	TYR	2.4
1	A	71	ASP	2.4
1	B	177	ARG	2.4
1	A	96	VAL	2.3
1	A	117	CYS	2.3
1	B	117	CYS	2.3
1	B	75	ARG	2.3
1	A	41	ALA	2.3
1	A	128	GLN	2.3
1	B	150	ARG	2.3
1	A	35	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	145	LEU	2.2
1	B	112	ILE	2.2
1	A	143	LEU	2.2
1	B	141	ILE	2.2
1	A	160	ALA	2.1
1	B	77	SER	2.1
1	A	109	ILE	2.1
1	B	96	VAL	2.1
1	B	121	ASP	2.1
1	A	115	HIS	2.1
1	A	15	GLN	2.0
1	A	144	ALA	2.0
1	B	160	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	QUE	A	1211	22/22	0.33	1.46	51,51,52,52	22
2	QUE	B	1211	22/22	0.26	0.40	63,64,64,64	22

## 6.5 Other polymers ⓘ

There are no such residues in this entry.