



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:16 pm BST

PDB ID : 3MFF  
Title : 1F1E8hu TCR  
Authors : van Boxel, G.I.; Holmes, S.; Fugger, L.; Jones, E.Y.  
Deposited on : 2010-04-02  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

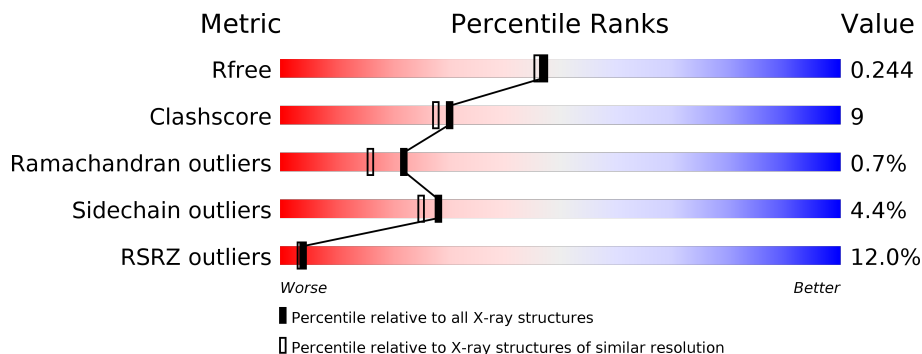
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . 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	200	 14% 81% 14% . .
1	C	200	 8% 81% 13% . . .
2	B	242	 14% 84% 14% .
2	D	242	 12% 83% 15% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7784 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.

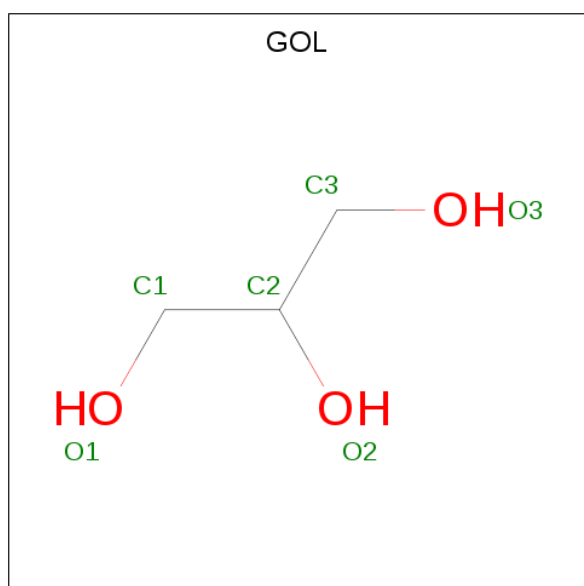
- Molecule 1 is a protein called T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	Total 1513	C 956	N 250	O 301	S 6	0	0	0
1	C	196	Total 1542	C 971	N 257	O 308	S 6	0	0	0

- Molecule 2 is a protein called T cell receptor beta chain.

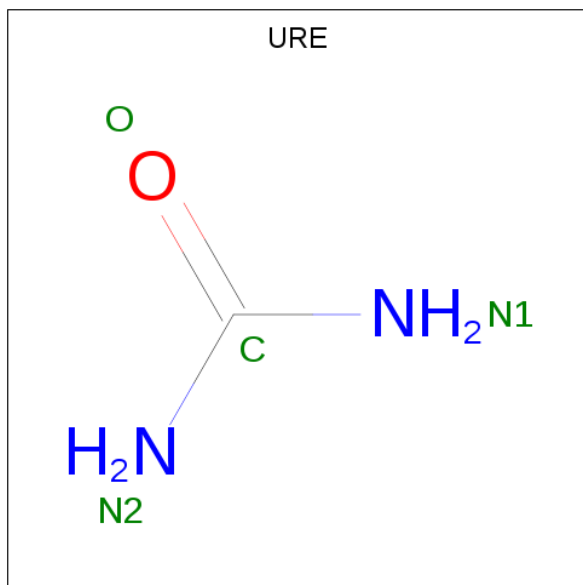
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	242	Total 1944	C 1225	N 337	O 373	S 9	0	0	0
2	D	242	Total 1948	C 1227	N 337	O 375	S 9	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



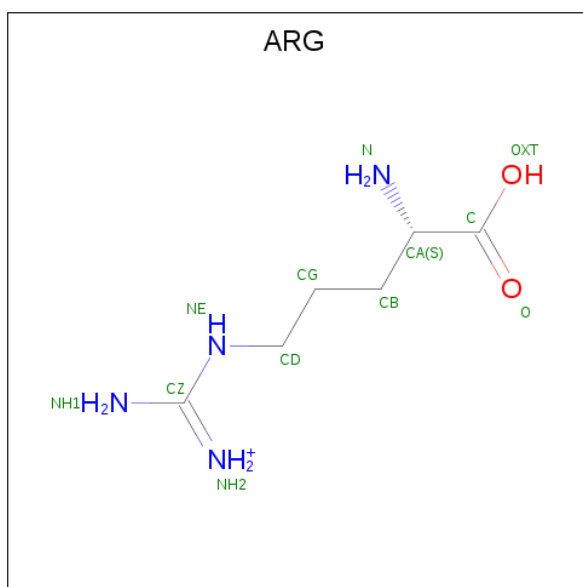
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is UREA (three-letter code: URE) (formula: CH<sub>4</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			4	1	2	1		
4	D	1	Total	C	N	O	0	0
			4	1	2	1		
4	D	1	Total	C	N	O	0	0
			4	1	2	1		

- Molecule 5 is ARGinine (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	D	1	11	6	4	1	0	0

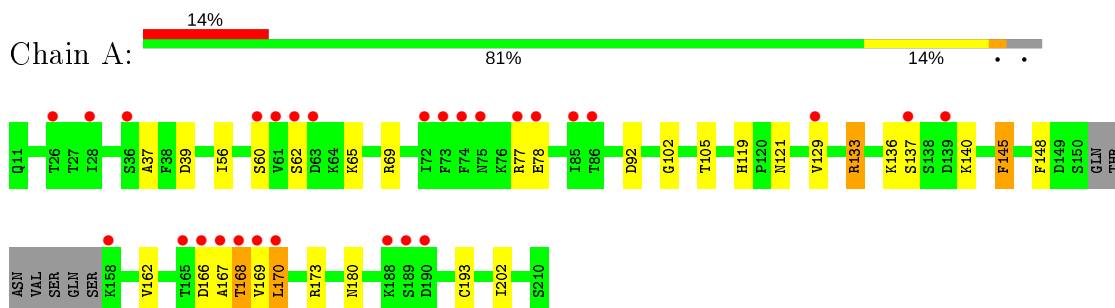
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	138	Total	O	0	0
			138	138		
6	B	243	Total	O	0	0
			243	243		
6	C	205	Total	O	0	0
			205	205		
6	D	216	Total	O	0	0
			216	216		

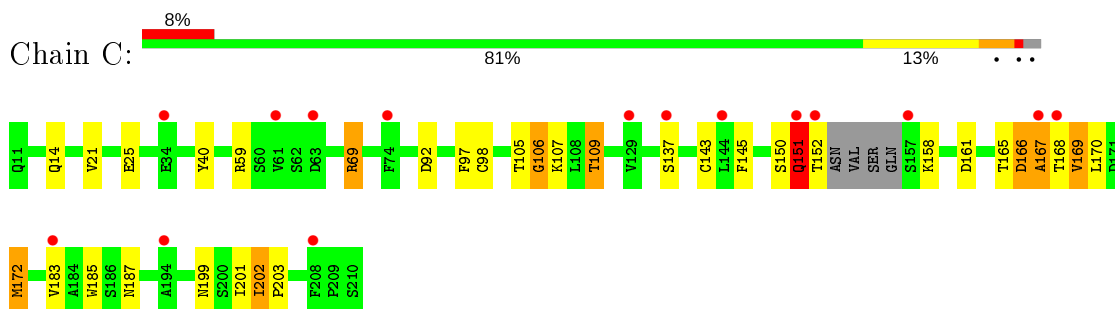
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

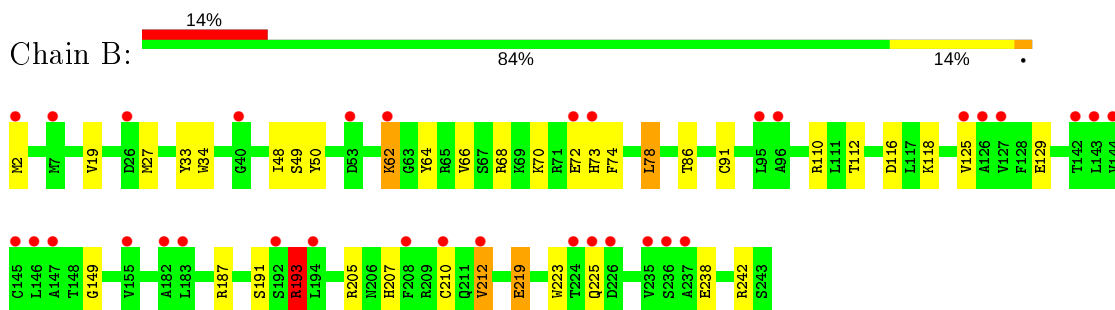
- Molecule 1: T cell receptor alpha chain



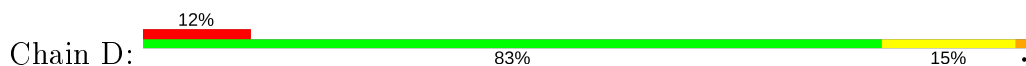
- Molecule 1: T cell receptor alpha chain

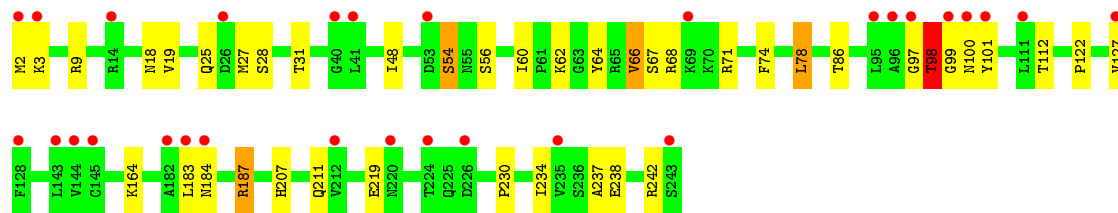


- Molecule 2: T cell receptor beta chain



- Molecule 2: T cell receptor beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.32Å 74.02Å 94.27Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.00-2.00) 91.7 (29.82-2.00)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.243 0.248 , 0.244	Depositor DCC
$R_{free}$ test set	3735 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.67	0/1551	0.72	1/2104 (0.0%)
1	C	0.67	0/1580	0.78	2/2142 (0.1%)
2	B	0.74	2/1995 (0.1%)	0.85	5/2708 (0.2%)
2	D	0.68	1/1999 (0.1%)	0.73	1/2713 (0.0%)
All	All	0.69	3/7125 (0.0%)	0.77	9/9667 (0.1%)

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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	ARG	CZ-NH1	10.52	1.46	1.33
2	B	210	CYS	CB-SG	-6.35	1.71	1.82
2	D	54	SER	CB-OG	6.29	1.50	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	ARG	NE-CZ-NH2	-14.32	113.14	120.30
2	B	68	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	C	69	ARG	NE-CZ-NH2	-9.75	115.43	120.30
2	B	193	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	C	69	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	B	68	ARG	NE-CZ-NH1	7.22	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	ARG	CG-CD-NE	-6.29	98.60	111.80
2	D	187	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	77	ARG	O-C-N	5.32	131.21	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	166	ASP	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	1513	0	1420	20	0
1	C	1542	0	1448	34	0
2	B	1944	0	1858	33	0
2	D	1948	0	1862	41	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
4	B	4	0	4	0	0
4	D	8	0	8	1	0
5	D	11	0	12	2	0
6	A	138	0	0	6	0
6	B	243	0	0	6	0
6	C	205	0	0	6	0
6	D	216	0	0	12	0
All	All	7784	0	6628	126	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 9.

All (126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ARG:NH1	2:D:71:ARG:HA	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:SER:O	1:C:151:GLN:HB2	1.67	0.93
2:D:99:GLY:HA2	2:D:101:TYR:N	1.83	0.93
2:B:242:ARG:HB2	6:B:273:HOH:O	1.71	0.91
2:D:99:GLY:HA2	2:D:101:TYR:H	1.36	0.91
1:A:162:VAL:HG23	1:A:202:ILE:HG22	1.51	0.91
1:C:166:ASP:HB3	1:C:167:ALA:HB3	1.54	0.89
1:A:162:VAL:HB	6:A:483:HOH:O	1.72	0.89
1:C:161:ASP:O	1:C:201:ILE:HD11	1.73	0.88
2:B:62:LYS:HD2	2:B:62:LYS:H	1.37	0.87
2:D:99:GLY:CA	2:D:101:TYR:H	1.91	0.84
2:D:68:ARG:HH12	2:D:71:ARG:HA	1.40	0.83
1:C:69:ARG:NH2	1:C:92:ASP:OD2	2.12	0.83
1:C:172:MET:SD	6:D:784:HOH:O	2.36	0.82
2:B:207:HIS:HD2	2:B:238:GLU:OE2	1.63	0.82
2:D:207:HIS:HD2	2:D:238:GLU:OE2	1.63	0.81
1:C:166:ASP:O	1:C:169:VAL:HG23	1.80	0.81
2:D:99:GLY:HA3	6:D:782:HOH:O	1.81	0.79
1:C:166:ASP:CB	1:C:167:ALA:HB3	2.13	0.79
1:C:199:ASN:HA	1:C:202:ILE:HD12	1.65	0.78
1:A:69:ARG:NH2	1:A:92:ASP:OD2	2.14	0.77
1:C:152:THR:HA	1:C:203:PRO:HA	1.67	0.76
2:B:66:VAL:CG1	2:B:74:PHE:CE1	2.69	0.76
1:A:166:ASP:HA	1:A:167:ALA:HB3	1.70	0.73
2:B:62:LYS:CD	2:B:62:LYS:H	1.99	0.73
2:D:164:LYS:HE2	6:D:478:HOH:O	1.87	0.73
2:B:70:LYS:HE3	6:B:738:HOH:O	1.88	0.71
2:D:66:VAL:CG1	2:D:74:PHE:CE1	2.74	0.71
2:D:219:GLU:HG3	6:D:295:HOH:O	1.93	0.69
2:B:66:VAL:HG11	2:B:74:PHE:CE1	2.29	0.68
2:B:66:VAL:HG13	2:B:74:PHE:CE1	2.29	0.68
2:B:66:VAL:CG1	2:B:74:PHE:HE1	2.05	0.67
1:A:39:ASP:HA	1:A:60:SER:HB2	1.76	0.67
2:D:207:HIS:CD2	2:D:238:GLU:OE2	2.48	0.66
2:D:66:VAL:HG13	2:D:74:PHE:CE1	2.31	0.65
2:D:62:LYS:HE3	2:D:64:TYR:HE2	1.61	0.65
2:B:191:SER:OG	2:B:193:ARG:NH2	2.28	0.65
2:D:2:MET:HB3	2:D:27:MET:HG2	1.78	0.64
1:C:172:MET:HG2	1:C:185:TRP:CZ2	2.34	0.62
2:D:66:VAL:HG11	2:D:74:PHE:CE1	2.34	0.62
2:B:207:HIS:CD2	2:B:238:GLU:OE2	2.51	0.61
2:D:2:MET:HG3	2:D:3:LYS:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASP:CA	1:C:167:ALA:HB3	2.31	0.61
2:D:66:VAL:CG1	2:D:74:PHE:HE1	2.13	0.60
1:A:105:THR:HG23	6:A:487:HOH:O	2.01	0.59
2:D:98:THR:HG21	6:D:785:HOH:O	2.03	0.59
2:D:60:ILE:O	2:D:62:LYS:HG3	2.03	0.57
2:B:219:GLU:HG2	6:B:368:HOH:O	2.02	0.57
2:D:242:ARG:HB2	6:D:703:HOH:O	2.03	0.57
1:A:166:ASP:CA	1:A:167:ALA:HB3	2.35	0.56
2:B:64:TYR:CD1	2:B:78:LEU:HD22	2.41	0.55
1:C:199:ASN:HA	1:C:202:ILE:CD1	2.35	0.55
1:C:14:GLN:NE2	1:C:98:CYS:H	2.06	0.54
2:B:48:ILE:HD13	2:B:50:TYR:CZ	2.43	0.54
1:C:107:LYS:HD3	2:D:48:ILE:HG21	1.90	0.53
2:D:98:THR:HG22	2:D:99:GLY:H	1.72	0.53
1:A:166:ASP:HA	1:A:167:ALA:CB	2.38	0.53
1:C:109:THR:HG22	6:C:312:HOH:O	2.07	0.53
1:C:105:THR:O	1:C:106:GLY:O	2.26	0.53
1:C:109:THR:HB	6:C:339:HOH:O	2.08	0.53
1:C:166:ASP:HB2	1:C:169:VAL:HG22	1.90	0.53
1:C:166:ASP:CA	1:C:167:ALA:CB	2.88	0.52
2:D:2:MET:HB3	2:D:27:MET:CG	2.40	0.52
2:D:62:LYS:HD2	6:D:635:HOH:O	2.10	0.52
2:B:86:THR:HG23	2:B:112:THR:HA	1.92	0.52
2:D:122:PRO:HD3	2:D:230:PRO:HB3	1.91	0.51
2:B:64:TYR:HD1	2:B:78:LEU:HD22	1.76	0.51
2:B:2:MET:HB2	2:B:27:MET:HG2	1.93	0.51
1:A:121:ASN:HB2	6:A:793:HOH:O	2.11	0.51
1:A:168:THR:O	1:A:170:LEU:HD12	2.12	0.50
1:C:21:VAL:HG13	1:C:25:GLU:HB2	1.94	0.49
1:C:166:ASP:HA	1:C:167:ALA:CB	2.43	0.49
2:D:60:ILE:HD12	2:D:62:LYS:HE2	1.95	0.48
2:D:219:GLU:CG	6:D:295:HOH:O	2.58	0.48
2:D:31:THR:OG1	2:D:97:GLY:HA2	2.13	0.48
2:B:33:TYR:O	2:B:91:CYS:HA	2.13	0.47
1:A:56:ILE:HD11	1:A:65:LYS:HG3	1.96	0.47
1:C:109:THR:CB	6:C:339:HOH:O	2.61	0.47
1:C:14:GLN:HE22	1:C:97:PHE:HA	1.80	0.47
1:C:40:TYR:HD1	1:C:59:ARG:HG2	1.78	0.47
2:D:62:LYS:HD3	6:D:410:HOH:O	2.14	0.47
1:C:151:GLN:HB3	1:C:152:THR:H	1.61	0.46
1:C:166:ASP:HB3	1:C:168:THR:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:THR:HG21	6:C:841:HOH:O	2.17	0.45
2:B:205:ARG:HG3	6:C:236:HOH:O	2.16	0.44
2:D:86:THR:HG23	2:D:112:THR:HA	1.99	0.44
2:B:223:TRP:NE1	2:B:225:GLN:HB2	2.32	0.44
1:A:37:ALA:O	1:A:102:GLY:HA3	2.16	0.44
1:C:166:ASP:HB3	1:C:168:THR:N	2.32	0.44
2:D:127:VAL:HG23	2:D:237:ALA:HB3	2.00	0.44
2:B:72:GLU:HG3	2:B:73:HIS:CD2	2.53	0.44
2:D:211:GLN:HG3	2:D:234:ILE:HG23	2.00	0.44
2:B:2:MET:HA	6:B:740:HOH:O	2.17	0.43
2:D:66:VAL:HG11	2:D:74:PHE:CZ	2.52	0.43
1:A:133:ARG:NH2	2:B:129:GLU:OE1	2.50	0.43
1:A:119:HIS:HB3	1:A:180:ASN:HD21	1.83	0.43
2:B:110:ARG:NH1	6:B:293:HOH:O	2.41	0.43
1:C:166:ASP:HA	1:C:167:ALA:HB3	2.01	0.43
2:D:187:ARG:HH22	4:D:245:URE:C	2.31	0.43
2:B:49:SER:HB2	2:B:74:PHE:CE1	2.54	0.43
2:B:78:LEU:HD23	2:B:78:LEU:N	2.33	0.43
2:D:60:ILE:O	2:D:62:LYS:CG	2.66	0.43
1:A:145:PHE:CE2	1:A:148:PHE:HA	2.53	0.42
2:B:116:ASP:OD1	2:B:118:LYS:HG2	2.18	0.42
1:C:168:THR:HB	6:C:607:HOH:O	2.19	0.42
2:D:9:ARG:H	5:D:246:ARG:HH22	1.67	0.42
2:B:223:TRP:CE2	2:B:225:GLN:HB2	2.54	0.42
1:A:140:LYS:HE2	1:A:140:LYS:HB3	1.85	0.42
2:B:66:VAL:HG11	2:B:74:PHE:CZ	2.54	0.42
1:C:143:CYS:O	1:C:183:VAL:HA	2.19	0.42
2:D:9:ARG:H	5:D:246:ARG:NH2	2.17	0.42
2:B:125:VAL:HG21	2:B:212:VAL:HG13	2.02	0.42
1:A:133:ARG:NH1	6:A:233:HOH:O	2.53	0.42
1:A:173:ARG:NH1	6:A:713:HOH:O	2.50	0.42
2:D:28:SER:HB2	6:D:651:HOH:O	2.20	0.41
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.92	0.41
2:D:219:GLU:HG2	6:D:497:HOH:O	2.20	0.41
2:D:64:TYR:CD1	2:D:78:LEU:HD22	2.55	0.41
1:C:165:THR:CG2	1:C:165:THR:O	2.68	0.41
2:B:149:GLY:O	2:B:187:ARG:HD2	2.21	0.41
2:D:18:ASN:OD1	6:D:269:HOH:O	2.21	0.41
1:A:133:ARG:HD3	6:A:233:HOH:O	2.21	0.40
2:B:34:TRP:HH2	6:B:333:HOH:O	2.03	0.40
1:A:129:VAL:HG11	1:A:193:CYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:HD13	2:B:50:TYR:OH	2.21	0.40
1:C:168:THR:O	1:C:168:THR:HG22	2.21	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	189/200 (94%)	179 (95%)	9 (5%)	1 (0%)	29	23
1	C	192/200 (96%)	186 (97%)	3 (2%)	3 (2%)	9	4
2	B	240/242 (99%)	234 (98%)	6 (2%)	0	100	100
2	D	240/242 (99%)	226 (94%)	12 (5%)	2 (1%)	19	13
All	All	861/884 (97%)	825 (96%)	30 (4%)	6 (1%)	22	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	106	GLY
1	C	151	GLN
2	D	98	THR
2	D	100	ASN
1	A	168	THR
1	C	167	ALA

### 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	168/177 (95%)	160 (95%)	8 (5%)	25	22
1	C	172/177 (97%)	163 (95%)	9 (5%)	23	19
2	B	214/215 (100%)	208 (97%)	6 (3%)	43	44
2	D	215/215 (100%)	205 (95%)	10 (5%)	26	22
All	All	769/784 (98%)	736 (96%)	33 (4%)	28	26

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	78	GLU
1	A	133	ARG
1	A	136	LYS
1	A	137	SER
1	A	145	PHE
1	A	169	VAL
1	A	170	LEU
2	B	19	VAL
2	B	62	LYS
2	B	78	LEU
2	B	193	ARG
2	B	212	VAL
2	B	219	GLU
1	C	109	THR
1	C	137	SER
1	C	145	PHE
1	C	151	GLN
1	C	158	LYS
1	C	169	VAL
1	C	172	MET
1	C	187	ASN
1	C	202	ILE
2	D	19	VAL
2	D	25	GLN
2	D	54	SER
2	D	56	SER
2	D	66	VAL
2	D	67	SER
2	D	78	LEU

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Mol	Chain	Res	Type
2	D	98	THR
2	D	183	LEU
2	D	184	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	180	ASN
2	B	55	ASN
2	B	73	HIS
2	B	103	GLN
2	B	207	HIS
1	C	14	GLN
1	C	180	ASN
2	D	55	ASN
2	D	100	ASN
2	D	207	HIS

### 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](#)

6 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
4	URE	D	244	-	3,3,3	0.24	0	3,3,3	1.29	0
3	GOL	A	2	-	5,5,5	0.39	0	5,5,5	0.21	0
3	GOL	D	1	-	5,5,5	0.48	0	5,5,5	0.63	0
4	URE	D	245	-	3,3,3	0.34	0	3,3,3	0.15	0
4	URE	B	244	-	3,3,3	0.41	0	3,3,3	0.64	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
3	GOL	A	2	-	-	1/4/4/4	-
3	GOL	D	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	GOL	O1-C1-C2-O2
3	D	1	GOL	O1-C1-C2-C3
3	A	2	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	245	URE	1	0

## 5.7 Other polymers [i](#)

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	193/200 (96%)	0.86	28 (14%) <b>2</b> <b>2</b>	27, 35, 44, 51	0
1	C	196/200 (98%)	0.59	15 (7%) <b>13</b> <b>12</b>	27, 35, 45, 56	0
2	B	242/242 (100%)	0.77	33 (13%) <b>3</b> <b>2</b>	28, 35, 46, 60	0
2	D	242/242 (100%)	0.91	29 (11%) <b>4</b> <b>3</b>	27, 34, 46, 61	0
All	All	873/884 (98%)	0.79	105 (12%) <b>4</b> <b>3</b>	27, 35, 46, 61	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	THR	9.2
2	D	96	ALA	7.8
1	A	167	ALA	6.7
2	D	99	GLY	6.3
1	C	152	THR	5.9
2	D	2	MET	5.7
2	B	224	THR	5.6
1	C	157	SER	5.4
2	D	224	THR	5.3
1	A	75	ASN	4.4
2	D	95	LEU	4.2
2	D	183	LEU	4.2
2	B	2	MET	4.1
1	A	74	PHE	3.9
2	D	182	ALA	3.8
1	A	166	ASP	3.8
1	A	61	VAL	3.8
2	B	95	LEU	3.7
1	A	137	SER	3.7
1	A	189	SER	3.7
1	A	63	ASP	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	170	LEU	3.5
1	A	190	ASP	3.5
2	B	127	VAL	3.4
2	B	145	CYS	3.4
2	B	183	LEU	3.4
2	D	184	ASN	3.4
2	B	212	VAL	3.4
2	D	97	GLY	3.4
2	D	101	TYR	3.4
1	A	78	GLU	3.3
1	C	151	GLN	3.3
1	A	73	PHE	3.3
2	D	41	LEU	3.2
2	B	126	ALA	3.2
2	B	235	VAL	3.2
1	C	168	THR	3.1
2	B	210	CYS	3.1
2	B	144	VAL	3.1
2	D	226	ASP	3.1
2	D	145	CYS	3.0
2	B	237	ALA	3.0
2	B	7	MET	3.0
2	D	26	ASP	3.0
2	D	144	VAL	3.0
2	B	226	ASP	3.0
1	C	137	SER	3.0
2	B	96	ALA	2.9
2	D	3	LYS	2.9
1	A	36	SER	2.9
2	B	125	VAL	2.9
2	D	220	ASN	2.8
1	A	86	THR	2.8
2	D	212	VAL	2.8
2	B	182	ALA	2.7
2	D	127	VAL	2.7
2	D	243	SER	2.7
2	B	146	LEU	2.7
2	B	194	LEU	2.7
1	A	158	LYS	2.7
1	C	34	GLU	2.7
1	A	169	VAL	2.6
2	B	53	ASP	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	40	GLY	2.6
1	C	74	PHE	2.6
1	A	60	SER	2.6
2	D	14	ARG	2.5
2	D	53	ASP	2.5
1	C	183	VAL	2.5
1	C	129	VAL	2.5
1	A	85	ILE	2.5
1	A	77	ARG	2.4
1	C	167	ALA	2.4
1	A	188	LYS	2.4
2	B	192	SER	2.4
2	B	143	LEU	2.4
2	D	111	LEU	2.4
2	D	69	LYS	2.4
2	D	100	ASN	2.4
1	C	208	PHE	2.4
2	B	208	PHE	2.3
2	D	128	PHE	2.3
1	C	194	ALA	2.3
1	A	62	SER	2.3
1	A	165	THR	2.3
2	B	40	GLY	2.3
2	B	236	SER	2.3
2	B	26	ASP	2.2
2	D	235	VAL	2.2
2	B	147	ALA	2.2
1	A	28	ILE	2.2
1	C	63	ASP	2.1
2	B	225	GLN	2.1
2	B	155	VAL	2.1
1	A	139	ASP	2.1
2	B	72	GLU	2.1
1	A	72	ILE	2.1
1	C	61	VAL	2.1
1	A	26	THR	2.1
2	B	142	THR	2.1
2	B	62	LYS	2.1
1	A	129	VAL	2.0
1	C	144	LEU	2.0
2	B	73	HIS	2.0
2	D	143	LEU	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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	URE	D	245	4/4	0.46	0.33	64,64,64,64	0
5	ARG	D	246	11/12	0.71	0.26	57,60,61,62	0
3	GOL	D	1	6/6	0.84	0.19	26,40,43,44	0
3	GOL	A	2	6/6	0.87	0.22	59,60,61,63	0
4	URE	B	244	4/4	0.88	0.15	37,38,38,38	0
4	URE	D	244	4/4	0.91	0.13	35,37,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.