



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MFF  
Title : 1F1E8hu TCR  
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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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

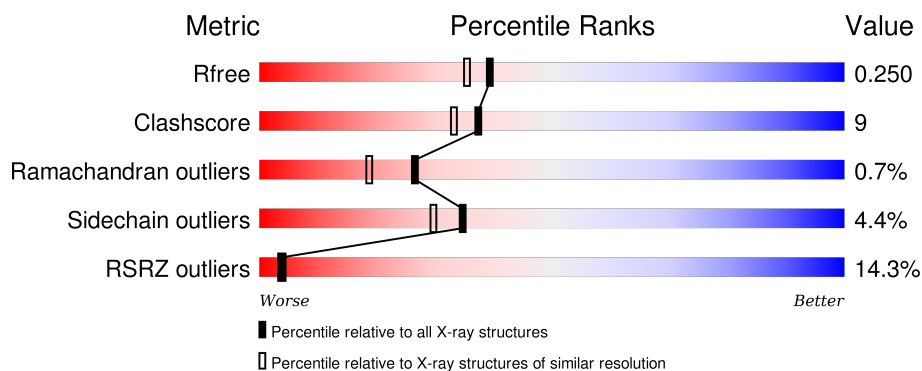
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>17%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	C	200	<div> <div>10%</div> <div>81%</div> <div>13%</div> <div>• • •</div> </div>
2	B	242	<div> <div>17%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
2	D	242	<div> <div>13%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ARG	D	246	-	-	-	X

## 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
1	A	193	Total	C	N	O	S	0	0	0
			1513	956	250	301	6			
1	C	196	Total	C	N	O	S	0	0	0
			1542	971	257	308	6			

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

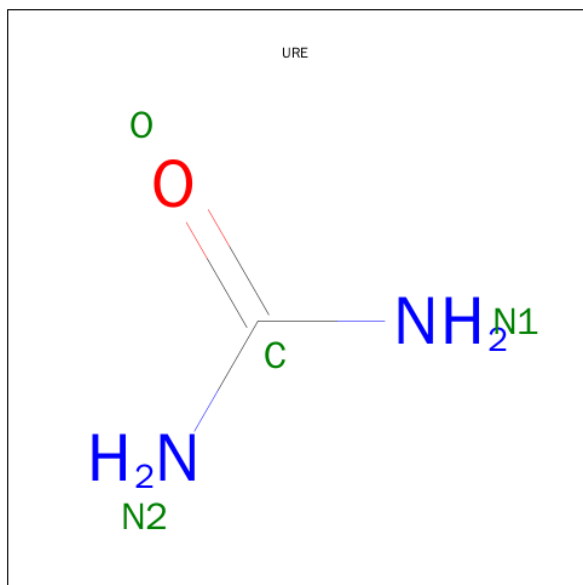
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1944	1225	337	373	9			
2	D	242	Total	C	N	O	S	0	0	0
			1948	1227	337	375	9			

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



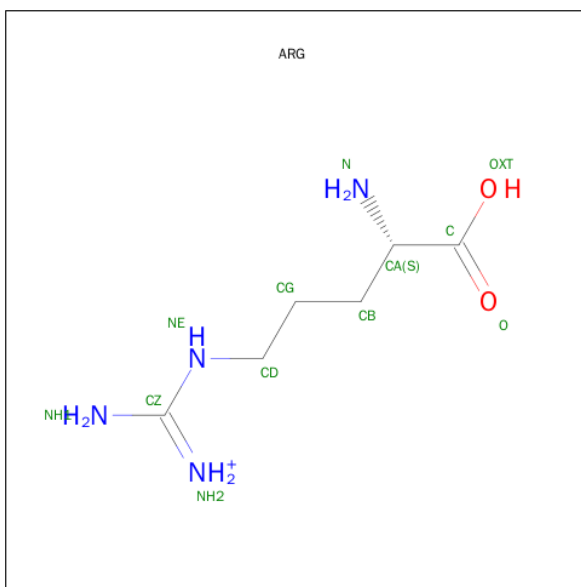
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is UREA (three-letter code: URE) (formula:  $\text{CH}_4\text{N}_2\text{O}$ ).



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:  $\text{C}_6\text{H}_{15}\text{N}_4\text{O}_2$ ).



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

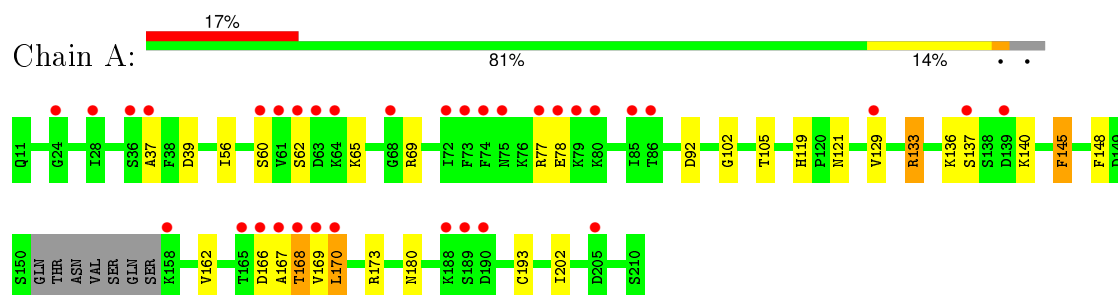
- Molecule 6 is water.

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		

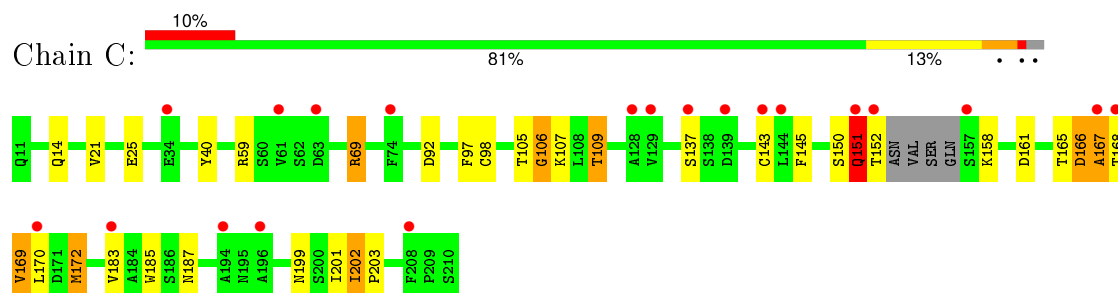
### 3 Residue-property plots [i](#)

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

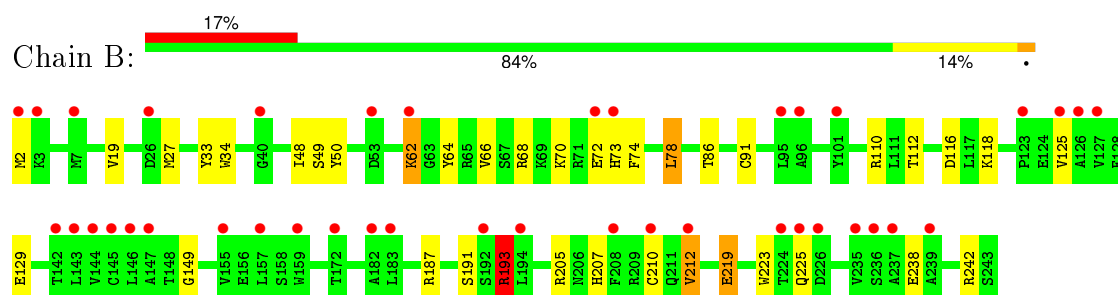
- Molecule 1: T cell receptor alpha chain



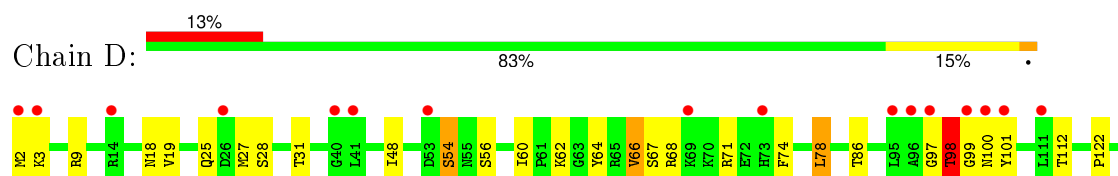
- Molecule 1: T cell receptor alpha chain

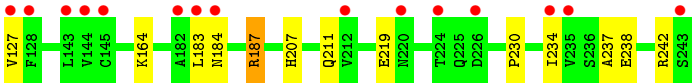


- Molecule 2: T cell receptor beta chain



- 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)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.243 0.249 , 0.250	Depositor DCC
$R_{free}$ test set	3735 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.5	EDS
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74561 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage'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, 0.375 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: 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

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
2:D:98:THR:HG22	2:D:99:GLY:H	1.72	0.53
1:C:107:LYS:HD3	2:D:48:ILE:HG21	1.90	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:166:ASP:HB2	1:C:169:VAL:HG22	1.90	0.53
1:C:109:THR:HB	6:C:339:HOH:O	2.08	0.53
1:C:105:THR:O	1:C:106:GLY:O	2.26	0.53
1:C:166:ASP:CA	1:C:167:ALA:CB	2.88	0.52
2:D:62:LYS:HD2	6:D:635:HOH:O	2.10	0.52
2:D:2:MET:HB3	2:D:27:MET:CG	2.40	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:C:109:THR:CB	6:C:339:HOH:O	2.61	0.47
1:A:56:ILE:HD11	1:A:65:LYS:HG3	1.96	0.47
1:C:14:GLN:HE22	1:C:97:PHE:HA	1.80	0.47
2:D:62:LYS:HD3	6:D:410:HOH:O	2.14	0.47
1:C:40:TYR:HD1	1:C:59:ARG:HG2	1.78	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: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
1:A:37:ALA:O	1:A:102:GLY:HA3	2.16	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:D:66:VAL:HG11	2:D:74:PHE:CZ	2.52	0.43
2:B:2:MET:HA	6:B:740:HOH:O	2.17	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:D:60:ILE:O	2:D:62:LYS:CG	2.66	0.43
2:B:78:LEU:HD23	2:B:78:LEU:N	2.33	0.43
1:C:168:THR:HB	6:C:607:HOH:O	2.19	0.42
2:B:116:ASP:OD1	2:B:118:LYS:HG2	2.18	0.42
1:A:145:PHE:CE2	1:A:148:PHE:HA	2.53	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
2:D:9:ARG:H	5:D:246:ARG:NH2	2.17	0.42
1:C:143:CYS:O	1:C:183:VAL:HA	2.19	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%)	34	26
1	C	192/200 (96%)	186 (97%)	3 (2%)	3 (2%)	12	5
2	B	240/242 (99%)	234 (98%)	6 (2%)	0	100	100
2	D	240/242 (99%)	226 (94%)	12 (5%)	2 (1%)	24	15
All	All	861/884 (97%)	825 (96%)	30 (4%)	6 (1%)	26	19

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%)	31	26
1	C	172/177 (97%)	163 (95%)	9 (5%)	29	23
2	B	214/215 (100%)	208 (97%)	6 (3%)	51	50
2	D	215/215 (100%)	205 (95%)	10 (5%)	32	27
All	All	769/784 (98%)	736 (96%)	33 (4%)	35	30

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	$\# Z  > 2$
3	GOL	A	2	-	5,5,5	0.35	0	5,5,5	0.19	0
4	URE	B	244	-	3,3,3	0.39	0	3,3,3	0.55	0
3	GOL	D	1	-	5,5,5	0.45	0	5,5,5	0.58	0
4	URE	D	244	-	3,3,3	0.24	0	3,3,3	1.14	0
4	URE	D	245	-	3,3,3	0.31	0	3,3,3	0.12	0
5	ARG	D	246	-	6,10,11	0.52	0	5,11,13	0.79	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	-	-	0/4/4/4	0/0/0/0
4	URE	B	244	-	-	0/0/0/0	0/0/0/0
3	GOL	D	1	-	-	0/4/4/4	0/0/0/0
4	URE	D	244	-	-	0/0/0/0	0/0/0/0
4	URE	D	245	-	-	0/0/0/0	0/0/0/0
5	ARG	D	246	-	-	0/5/9/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	245	URE	1	0
5	D	246	ARG	2	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<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%)	0.93	34 (17%) 2 2	27, 35, 44, 51	0
1	C	196/200 (98%)	0.66	20 (10%) 9 9	27, 35, 45, 56	0
2	B	242/242 (100%)	0.84	40 (16%) 2 3	28, 35, 46, 60	0
2	D	242/242 (100%)	0.99	31 (12%) 5 5	27, 34, 46, 61	0
All	All	873/884 (98%)	0.86	125 (14%) 4 4	27, 35, 46, 61	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	THR	9.6
2	D	96	ALA	7.9
1	A	167	ALA	7.0
2	D	99	GLY	6.8
1	C	152	THR	6.7
2	D	2	MET	5.8
1	C	157	SER	5.7
2	B	224	THR	5.7
2	D	224	THR	5.3
2	D	95	LEU	4.6
1	A	75	ASN	4.6
2	D	183	LEU	4.4
1	A	74	PHE	4.4
2	D	182	ALA	4.3
1	A	61	VAL	4.3
1	A	189	SER	4.1
2	B	2	MET	4.0
1	A	166	ASP	3.9
1	A	190	ASP	3.8
2	D	97	GLY	3.8
2	B	127	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	212	VAL	3.7
2	B	95	LEU	3.7
1	A	137	SER	3.7
2	B	145	CYS	3.7
2	D	101	TYR	3.6
1	A	63	ASP	3.6
1	A	78	GLU	3.5
2	B	126	ALA	3.4
2	D	184	ASN	3.4
1	A	73	PHE	3.4
2	B	144	VAL	3.4
1	A	170	LEU	3.4
2	B	183	LEU	3.4
2	B	235	VAL	3.3
1	C	168	THR	3.3
2	B	237	ALA	3.3
2	B	210	CYS	3.3
2	D	144	VAL	3.3
1	C	151	GLN	3.3
2	D	41	LEU	3.3
2	B	7	MET	3.2
1	C	137	SER	3.2
2	B	226	ASP	3.2
2	D	145	CYS	3.2
2	D	26	ASP	3.1
2	D	226	ASP	3.1
2	B	125	VAL	3.1
1	A	169	VAL	3.0
2	D	3	LYS	3.0
1	A	36	SER	3.0
2	B	182	ALA	3.0
2	D	220	ASN	3.0
1	C	74	PHE	2.9
2	D	127	VAL	2.9
2	B	194	LEU	2.9
2	D	40	GLY	2.8
1	A	60	SER	2.8
1	A	86	THR	2.8
2	D	212	VAL	2.8
1	A	158	LYS	2.8
2	B	53	ASP	2.8
2	D	14	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	96	ALA	2.8
2	D	53	ASP	2.8
2	B	146	LEU	2.8
1	C	34	GLU	2.7
1	C	167	ALA	2.7
2	D	243	SER	2.7
1	C	129	VAL	2.6
1	C	183	VAL	2.6
2	B	143	LEU	2.5
1	C	208	PHE	2.5
2	B	208	PHE	2.5
2	D	128	PHE	2.5
1	A	85	ILE	2.5
2	B	192	SER	2.5
2	B	26	ASP	2.5
1	A	77	ARG	2.5
1	A	188	LYS	2.5
2	D	111	LEU	2.4
1	C	194	ALA	2.4
2	D	100	ASN	2.4
1	A	139	ASP	2.4
2	D	235	VAL	2.4
1	A	62	SER	2.4
2	D	69	LYS	2.4
1	A	165	THR	2.3
2	B	147	ALA	2.3
1	A	28	ILE	2.3
2	B	236	SER	2.3
1	C	63	ASP	2.3
2	B	142	THR	2.3
2	B	72	GLU	2.3
2	B	155	VAL	2.2
2	B	40	GLY	2.2
1	C	139	ASP	2.2
1	A	72	ILE	2.2
1	A	37	ALA	2.2
1	C	196	ALA	2.2
1	C	61	VAL	2.2
1	A	68	GLY	2.2
2	B	157	LEU	2.1
1	A	24	GLY	2.1
1	C	143	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	225	GLN	2.1
2	D	73	HIS	2.1
2	D	143	LEU	2.1
2	B	239	ALA	2.1
2	D	234	ILE	2.1
1	A	64	LYS	2.1
2	B	159	TRP	2.1
1	A	129	VAL	2.1
1	A	79	LYS	2.1
1	C	144	LEU	2.1
2	B	73	HIS	2.1
2	B	101	TYR	2.1
1	A	80	LYS	2.1
2	B	3	LYS	2.1
1	C	170	LEU	2.1
1	C	128	ALA	2.1
2	B	62	LYS	2.0
2	B	172	THR	2.0
2	B	123	PRO	2.0
1	A	205	ASP	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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	ARG	D	246	11/12	0.70	0.26	3.04	57,60,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	2	6/6	0.86	0.22	1.41	59,60,61,63	0
3	GOL	D	1	6/6	0.84	0.18	0.75	26,40,43,44	0
4	URE	B	244	4/4	0.89	0.14	-0.01	37,38,38,38	0
4	URE	D	244	4/4	0.91	0.13	-1.01	35,37,38,39	0
4	URE	D	245	4/4	0.47	0.33	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.