Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2017 – 05:41 PM EST

PDB ID	:	5JHD
Title	:	Crystal structure of LS10-TCR/M1-HLA-A*02 complex
Authors	:	Stern, L.J.; Selin, L.K.; Song, I.
Deposited on	:	2016-04-20
Resolution	:	2.46 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:

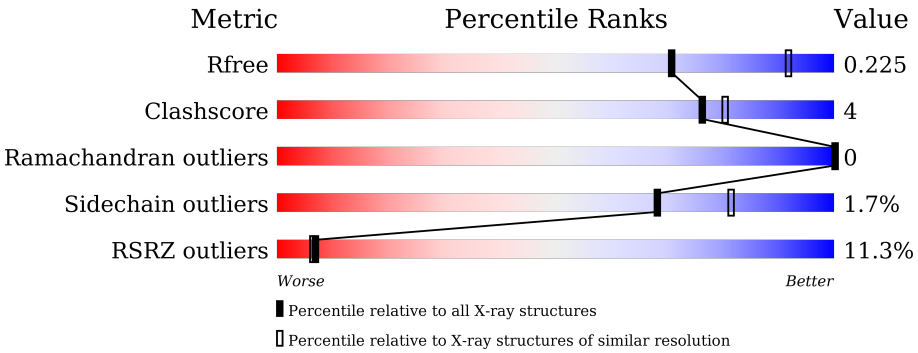
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.46 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.



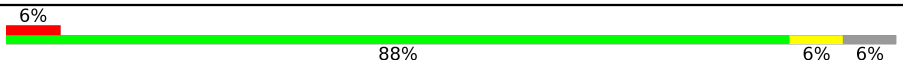
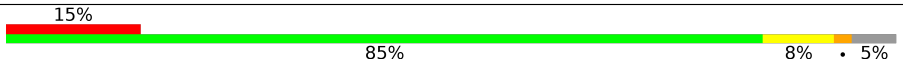
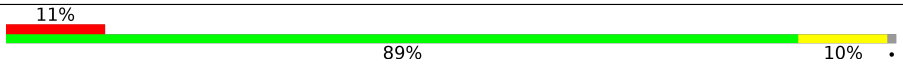
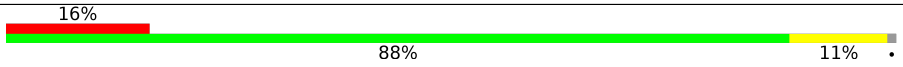
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	276	13% 91% 8%
1	F	276	12% 90% 10%
2	B	100	4% 95% 5%
2	G	100	3% 93% 7%
3	C	9	89% 11%
3	H	9	89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	213	
4	I	213	
5	E	242	
5	J	242	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDT	E	301	-	-	-	X
6	EDT	J	301	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26038 atoms, of which 12546 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	H	N	O	S	0	2	0
			4378	1412	2115	414	428	9			
1	F	276	Total	C	H	N	O	S	0	1	0
			4339	1403	2091	409	427	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	ALA	-	expression tag	UNP P01892
F	276	ALA	-	expression tag	UNP P01892

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	100	Total	C	H	N	O	S	0	0	0
			1625	530	792	140	159	4			
2	G	100	Total	C	H	N	O	S	0	0	0
			1625	530	792	140	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Influenza M1(58-66) peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O	0	0	0
			144	49	75	9	11			
3	H	9	Total	C	H	N	O	0	0	0
			144	49	75	9	11			

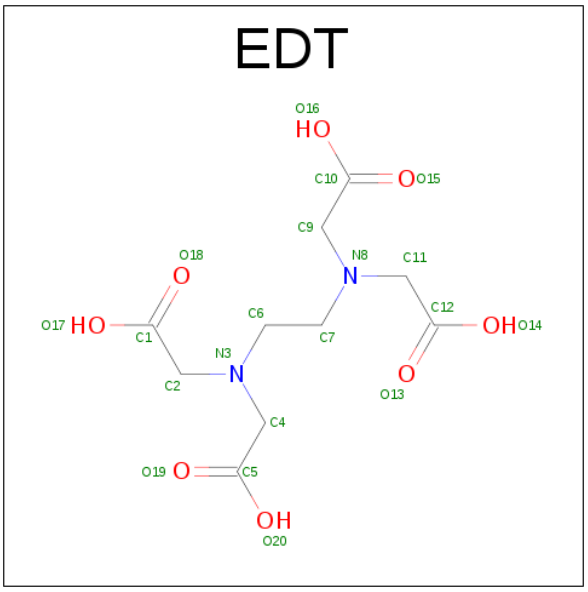
- Molecule 4 is a protein called TCRalpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	201	Total	C	H	N	O	S	0	0	0
			3078	995	1494	259	320	10			
4	I	203	Total	C	H	N	O	S	0	0	0
			3099	1003	1501	262	323	10			

- Molecule 5 is a protein called TCRbeta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	239	Total	C	H	N	O	S	0	0	0
			3691	1202	1793	327	363	6			
5	J	239	Total	C	H	N	O	S	0	0	0
			3692	1202	1794	327	363	6			

- Molecule 6 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	H	N	O	0	0
			32	10	12	2	8		
6	J	1	Total	C	H	N	O	0	0
			32	10	12	2	8		

- Molecule 7 is water.

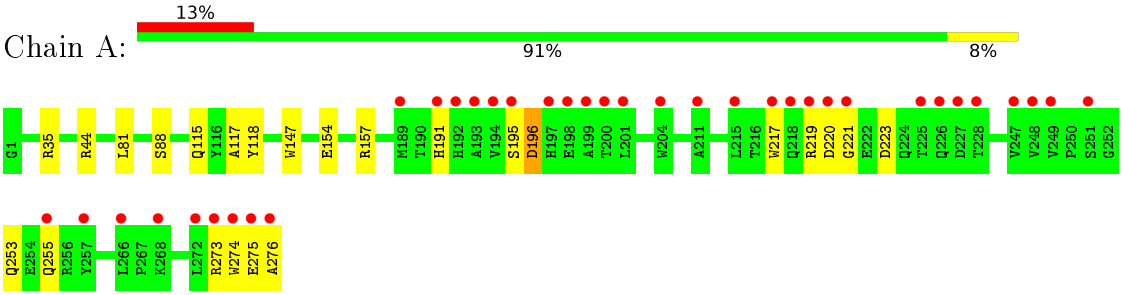
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	34	Total O 34 34	0	0
7	B	13	Total O 13 13	0	0
7	C	3	Total O 3 3	0	0
7	D	17	Total O 17 17	0	0
7	E	12	Total O 12 12	0	0
7	F	40	Total O 40 40	0	0
7	G	13	Total O 13 13	0	0
7	I	13	Total O 13 13	0	0
7	J	14	Total O 14 14	0	0

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.

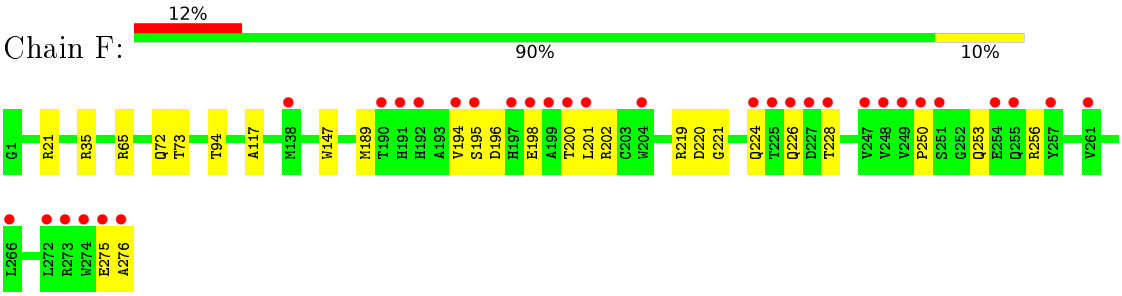
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



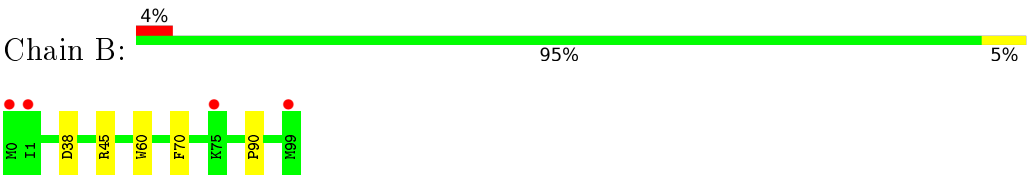
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:



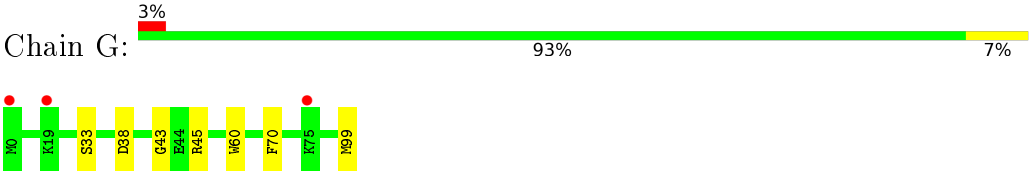
- Molecule 2: Beta-2-microglobulin

Chain B:



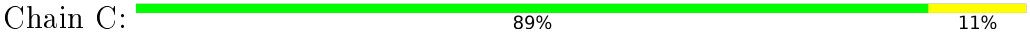
- Molecule 2: Beta-2-microglobulin

Chain G:



- Molecule 3: Influenza M1(58-66) peptide

Chain C:

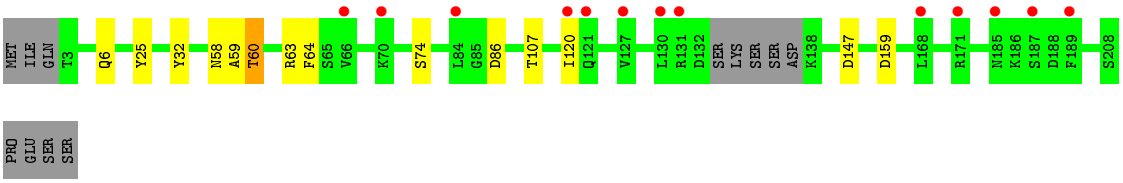


• Molecule 3: Influenza M1(58-66) peptide

Chain H:

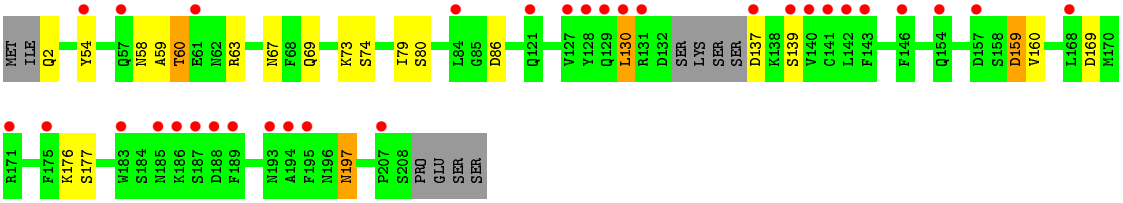
• Molecule 4: TCRalpha chain

Chain D:



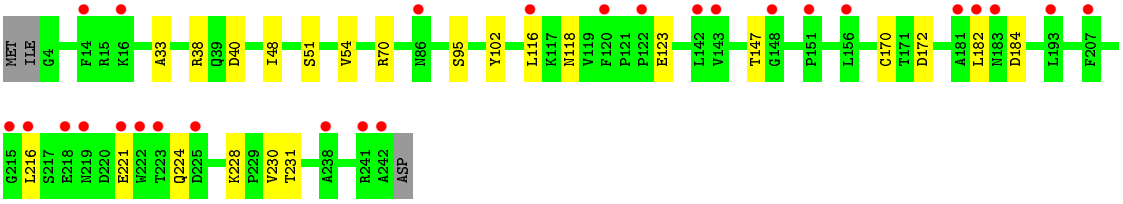
• Molecule 4: TCRalpha chain

Chain I:



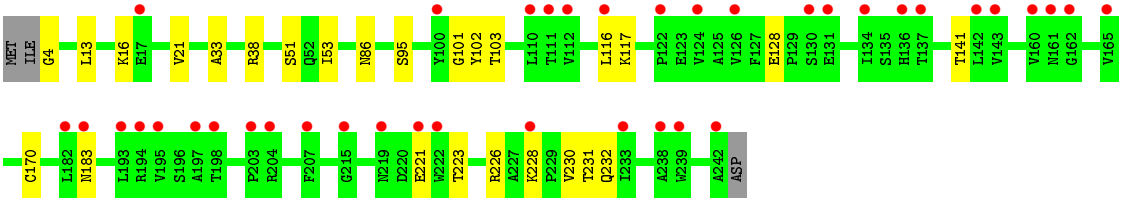
• Molecule 5: TCRbeta chain

Chain E:



• Molecule 5: TCRbeta chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.71Å 101.84Å 113.55Å 99.38° 92.60° 103.45°	Depositor
Resolution (Å)	29.05 – 2.46 80.92 – 2.46	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.05-2.46) 85.0 (80.92-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.223 0.203 , 0.225	Depositor DCC
R_{free} test set	3359 reflections (4.91%)	DCC
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26038	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: EDT

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	0.26	0/2333	0.46	0/3165
1	F	0.27	0/2318	0.46	0/3147
2	B	0.27	0/856	0.46	0/1158
2	G	0.28	0/856	0.46	0/1158
3	C	0.39	0/70	0.52	0/92
3	H	0.41	0/70	0.47	0/92
4	D	0.30	0/1619	0.49	0/2196
4	I	0.29	0/1633	0.48	0/2215
5	E	0.32	1/1950 (0.1%)	0.47	0/2656
5	J	0.32	1/1950 (0.1%)	0.45	0/2656
All	All	0.29	2/13655 (0.0%)	0.47	0/18535

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	228	LYS	C-N	7.82	1.49	1.34
5	J	228	LYS	C-N	7.18	1.47	1.34

There are no bond angle outliers.

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	2263	2115	2109	20	0
1	F	2248	2091	2085	20	0
2	B	833	792	792	2	1
2	G	833	792	792	6	0
3	C	69	75	75	1	0
3	H	69	75	75	1	0
4	D	1584	1494	1492	9	0
4	I	1598	1501	1502	19	0
5	E	1898	1793	1793	13	0
5	J	1898	1794	1794	14	0
6	E	20	12	12	0	0
6	J	20	12	12	1	1
7	A	34	0	0	5	0
7	B	13	0	0	0	0
7	C	3	0	0	0	0
7	D	17	0	0	2	0
7	E	12	0	0	4	0
7	F	40	0	0	7	0
7	G	13	0	0	3	0
7	I	13	0	0	8	0
7	J	14	0	0	2	0
All	All	13492	12546	12533	99	1

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 4.

All (99) 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)
4:D:6:GLN:O	7:D:301:HOH:O	1.82	0.96
4:I:2:GLN:OE1	7:I:301:HOH:O	1.85	0.94
5:J:4:GLY:N	7:J:401:HOH:O	2.02	0.91
5:E:147:THR:O	7:E:401:HOH:O	1.95	0.83
4:D:74:SER:OG	7:D:302:HOH:O	1.98	0.82
4:I:160:VAL:N	7:I:305:HOH:O	2.13	0.81
4:I:137:ASP:O	7:I:302:HOH:O	1.99	0.81
1:F:21:ARG:NE	7:F:301:HOH:O	2.06	0.77
4:I:74:SER:OG	7:I:303:HOH:O	2.02	0.76
5:E:123:GLU:N	7:E:401:HOH:O	2.19	0.75
4:I:139:SER:O	7:I:304:HOH:O	2.06	0.74
1:F:224:GLN:O	7:F:302:HOH:O	2.06	0.72
4:D:25:TYR:HH	4:D:32:TYR:HH	1.27	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:123:GLU:O	7:E:401:HOH:O	2.08	0.69
1:A:154:GLU:HG3	7:A:320:HOH:O	1.93	0.69
2:G:38:ASP:OD1	7:G:101:HOH:O	2.10	0.68
1:A:115:GLN:NE2	7:A:304:HOH:O	2.29	0.65
2:G:43:GLY:N	7:G:103:HOH:O	2.22	0.64
5:E:221:GLU:N	5:E:221:GLU:OE2	2.31	0.63
4:I:59:ALA:HB1	4:I:60:THR:HA	1.80	0.62
5:J:38:ARG:NH2	5:J:86:ASN:O	2.32	0.62
5:J:221:GLU:N	5:J:221:GLU:OE1	2.33	0.61
1:A:253:GLN:OE1	1:A:253:GLN:N	2.33	0.61
1:F:226:GLN:O	7:F:302:HOH:O	2.16	0.60
1:F:253:GLN:OE1	1:F:253:GLN:N	2.34	0.60
1:F:220:ASP:N	1:F:221:GLY:HA3	2.18	0.58
1:A:220:ASP:N	1:A:221:GLY:HA3	2.20	0.57
4:D:59:ALA:HB1	4:D:60:THR:HA	1.86	0.57
4:I:79:ILE:HA	7:I:307:HOH:O	2.06	0.55
4:I:63:ARG:NH2	4:I:86:ASP:OD2	2.39	0.55
5:J:117:LYS:O	5:J:226:ARG:NH2	2.40	0.54
4:I:159:ASP:OD1	4:I:159:ASP:N	2.41	0.54
4:I:59:ALA:HB1	4:I:60:THR:HG23	1.88	0.54
1:F:65:ARG:NH2	7:F:307:HOH:O	2.41	0.53
4:I:197:ASN:ND2	4:I:197:ASN:O	2.37	0.53
1:F:72:GLN:HG3	7:F:303:HOH:O	2.09	0.52
2:G:38:ASP:OD1	2:G:45:ARG:NE	2.43	0.52
1:F:94:THR:OG1	7:F:304:HOH:O	2.19	0.51
4:I:130:LEU:HD12	4:I:130:LEU:N	2.27	0.49
4:I:58:ASN:O	4:I:59:ALA:HB3	2.12	0.49
4:D:58:ASN:O	4:D:59:ALA:HB3	2.12	0.49
1:F:202:ARG:NE	2:G:99:MET:O	2.42	0.47
4:I:69:GLN:O	4:I:73:LYS:N	2.48	0.46
1:A:191:HIS:HB2	1:A:274:TRP:CH2	2.50	0.46
1:A:274:TRP:CD2	1:A:275:GLU:HA	2.50	0.46
1:F:228:THR:HB	7:F:302:HOH:O	2.15	0.46
1:A:157[A]:ARG:NH1	7:A:309:HOH:O	2.48	0.46
1:F:195:SER:O	1:F:196:ASP:C	2.53	0.46
6:J:301:EDT:H041	7:J:409:HOH:O	2.16	0.45
1:A:275:GLU:HG3	1:A:276:ALA:N	2.32	0.45
4:I:67:ASN:O	7:I:303:HOH:O	2.21	0.45
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.52	0.45
4:I:169:ASP:OD2	4:I:176:LYS:NZ	2.50	0.44
1:A:255:GLN:O	1:A:273:ARG:NH2	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:MET:HE2	1:F:201:LEU:HD22	1.98	0.44
1:F:198:GLU:HA	1:F:250:PRO:HA	2.00	0.44
5:E:118:ASN:ND2	5:E:184:ASP:OD2	2.50	0.44
1:F:147:TRP:CZ2	3:H:9:LEU:HD23	2.53	0.43
5:E:116:LEU:HD11	5:E:216:LEU:HD21	1.99	0.43
1:A:44:ARG:NH1	7:A:310:HOH:O	2.51	0.43
1:A:274:TRP:CE3	1:A:275:GLU:HA	2.53	0.43
1:A:196:ASP:OD2	1:A:196:ASP:N	2.50	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
5:E:33:ALA:HA	5:E:51:SER:O	2.18	0.43
4:D:63:ARG:NH2	4:D:86:ASP:OD2	2.52	0.43
5:E:116:LEU:HD13	5:E:116:LEU:O	2.19	0.43
5:J:230:VAL:O	5:J:232:GLN:HG2	2.19	0.43
1:F:194:VAL:CG2	1:F:200:THR:HG23	2.49	0.43
1:F:275:GLU:HG3	1:F:276:ALA:N	2.34	0.43
1:A:275:GLU:O	1:A:276:ALA:HB2	2.19	0.43
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.54	0.42
5:J:33:ALA:HA	5:J:51:SER:O	2.19	0.42
4:I:59:ALA:HB1	4:I:60:THR:CA	2.48	0.42
4:D:60:THR:HG21	4:D:64:PHE:O	2.19	0.42
5:J:183:ASN:OD1	5:J:183:ASN:N	2.53	0.42
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.54	0.41
4:D:59:ALA:HB1	4:D:60:THR:CA	2.50	0.41
5:E:54:VAL:HG23	5:E:70:ARG:O	2.19	0.41
5:J:13:LEU:HD21	5:J:21:VAL:HG11	2.02	0.41
4:D:120:ILE:CD1	4:D:147:ASP:HA	2.50	0.41
5:J:230:VAL:HG12	5:J:231:THR:N	2.35	0.41
5:E:172:ASP:OD2	7:E:402:HOH:O	2.22	0.41
5:E:38:ARG:NH2	5:E:40:ASP:OD2	2.53	0.41
5:J:101:GLY:O	5:J:103:THR:HG23	2.20	0.41
2:G:33:SER:OG	7:G:102:HOH:O	2.13	0.41
2:B:38:ASP:OD1	2:B:45:ARG:NE	2.53	0.41
4:I:130:LEU:HB3	5:J:128:GLU:O	2.20	0.41
1:A:195:SER:OG	1:A:196:ASP:OD2	2.37	0.41
5:J:16:LYS:HE3	5:J:116:LEU:HD11	2.02	0.41
5:J:223:THR:HG22	5:J:223:THR:O	2.21	0.41
1:F:73:THR:HA	5:J:53:ILE:HD13	2.03	0.41
1:A:274:TRP:HA	1:A:275:GLU:HA	1.86	0.41
1:A:217:TRP:O	1:A:223:ASP:HA	2.21	0.41
1:A:88:SER:O	7:A:301:HOH:O	2.22	0.40
5:E:230:VAL:HG22	5:E:231:THR:N	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:ASP:OD2	1:F:256:ARG:NH2	2.54	0.40
5:E:38:ARG:HB2	5:E:48:ILE:HD11	2.03	0.40
1:F:194:VAL:HG23	1:F:200:THR:HG23	2.03	0.40
4:I:80:SER:N	7:I:307:HOH:O	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PRO:O	6:J:301:EDT:O13[1_655]	1.27	0.93

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	276/276 (100%)	267 (97%)	9 (3%)	0	100	100
1	F	275/276 (100%)	266 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	G	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	197/213 (92%)	191 (97%)	6 (3%)	0	100	100
4	I	199/213 (93%)	193 (97%)	6 (3%)	0	100	100
5	E	237/242 (98%)	229 (97%)	8 (3%)	0	100	100
5	J	237/242 (98%)	230 (97%)	7 (3%)	0	100	100
All	All	1631/1680 (97%)	1581 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	232/231 (100%)	229 (99%)	3 (1%)	76 86
1	F	230/231 (100%)	228 (99%)	2 (1%)	84 91
2	B	94/95 (99%)	93 (99%)	1 (1%)	80 88
2	G	94/95 (99%)	93 (99%)	1 (1%)	80 88
3	C	7/7 (100%)	7 (100%)	0	100 100
3	H	7/7 (100%)	7 (100%)	0	100 100
4	D	179/191 (94%)	176 (98%)	3 (2%)	68 81
4	I	180/191 (94%)	174 (97%)	6 (3%)	45 61
5	E	204/210 (97%)	199 (98%)	5 (2%)	55 72
5	J	204/210 (97%)	200 (98%)	4 (2%)	63 78
All	All	1431/1468 (98%)	1406 (98%)	25 (2%)	68 81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	196	ASP
1	A	219	ARG
2	B	70	PHE
4	D	60	THR
4	D	107	THR
4	D	159	ASP
5	E	95	SER
5	E	102	TYR
5	E	170	CYS
5	E	182	LEU
5	E	224	GLN
1	F	35	ARG
1	F	219	ARG
2	G	70	PHE
4	I	54	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	60	THR
4	I	130	LEU
4	I	159	ASP
4	I	177	SER
4	I	197	ASN
5	J	95	SER
5	J	102	TYR
5	J	141	THR
5	J	170	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
6	EDT	E	301	-	7,19,19	0.35	0	12,24,24	2.32	6 (50%)
6	EDT	J	301	-	7,19,19	0.33	0	12,24,24	1.84	3 (25%)

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
6	EDT	E	301	-	-	0/13/21/21	0/0/0/0
6	EDT	J	301	-	-	0/13/21/21	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	301	EDT	C10-C9-N8	-4.22	107.27	113.53
6	J	301	EDT	C10-C9-N8	-3.48	108.38	113.53
6	E	301	EDT	C1-C2-N3	-3.35	108.57	113.53
6	J	301	EDT	C1-C2-N3	-2.79	109.40	113.53
6	E	301	EDT	C5-C4-N3	-2.69	109.55	113.53
6	J	301	EDT	C11-N8-C7	-2.18	106.64	111.26
6	E	301	EDT	C6-C7-N8	-2.10	107.89	113.13
6	E	301	EDT	C11-N8-C9	2.53	115.05	110.77
6	E	301	EDT	C11-N8-C7	3.55	118.80	111.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	301	EDT	1	1

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	276/276 (100%)	0.85	36 (13%) 5 4	26, 52, 130, 149	0
1	F	276/276 (100%)	0.95	32 (11%) 6 6	27, 50, 135, 190	0
2	B	100/100 (100%)	0.52	4 (4%) 42 45	24, 37, 74, 100	0
2	G	100/100 (100%)	0.45	3 (3%) 54 57	24, 40, 76, 98	0
3	C	9/9 (100%)	0.64	0 100 100	34, 39, 43, 45	0
3	H	9/9 (100%)	0.81	0 100 100	35, 37, 42, 46	0
4	D	201/213 (94%)	0.78	13 (6%) 22 24	45, 71, 111, 143	0
4	I	203/213 (95%)	1.08	32 (15%) 3 2	35, 84, 122, 135	0
5	E	239/242 (98%)	0.92	27 (11%) 7 6	37, 72, 122, 144	0
5	J	239/242 (98%)	1.12	39 (16%) 2 2	30, 75, 127, 157	0
All	All	1652/1680 (98%)	0.89	186 (11%) 7 6	24, 62, 124, 190	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	276	ALA	8.4
1	F	274	TRP	7.1
1	F	198	GLU	6.1
5	J	239	TRP	6.1
1	A	274	TRP	5.5
5	J	182	LEU	5.4
5	E	216	LEU	5.4
5	E	215	GLY	5.3
1	A	276	ALA	5.1
4	I	157	ASP	5.1
1	F	194	VAL	5.0
4	I	139	SER	5.0
1	F	257	TYR	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	I	130	LEU	4.8
1	F	195	SER	4.7
1	A	191	HIS	4.6
1	F	254	GLU	4.6
5	J	162	GLY	4.6
5	J	195	VAL	4.3
1	A	195	SER	4.3
1	F	275	GLU	4.2
5	J	203	PRO	4.2
4	I	140	VAL	4.2
5	E	222	TRP	4.2
5	J	242	ALA	4.2
1	A	272	LEU	4.2
5	E	221	GLU	4.2
1	F	249	VAL	4.1
1	F	227	ASP	3.9
1	F	255	GLN	3.8
1	F	199	ALA	3.8
1	F	228	THR	3.8
5	E	14	PHE	3.8
1	F	273	ARG	3.8
1	F	201	LEU	3.8
2	B	0	MET	3.8
1	A	249	VAL	3.7
4	I	207	PRO	3.7
5	J	126	VAL	3.7
1	F	197	HIS	3.6
1	F	226	GLN	3.6
4	I	189	PHE	3.6
5	E	182	LEU	3.5
4	D	187	SER	3.5
4	I	185	ASN	3.5
1	F	248	VAL	3.5
4	D	185	ASN	3.5
4	D	189	PHE	3.4
1	A	199	ALA	3.4
1	F	191	HIS	3.4
1	A	201	LEU	3.4
5	J	116	LEU	3.4
5	J	130	SER	3.4
5	E	241	ARG	3.4
1	A	255	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	3.3
5	J	221	GLU	3.3
1	F	247	VAL	3.3
1	A	247	VAL	3.3
4	I	194	ALA	3.3
4	I	142	LEU	3.3
1	A	248	VAL	3.3
1	A	215	LEU	3.2
5	J	219	ASN	3.2
1	A	211	ALA	3.2
1	A	220	ASP	3.2
5	J	193	LEU	3.2
4	I	187	SER	3.2
5	E	122	PRO	3.2
1	F	261	VAL	3.1
1	A	257	TYR	3.1
5	E	225	ASP	3.1
4	I	186	LYS	3.1
1	F	192	HIS	3.1
1	A	194	VAL	3.1
5	J	142	LEU	3.1
5	J	207	PHE	3.1
5	E	242	ALA	3.1
5	J	238	ALA	3.0
4	D	70	LYS	3.0
5	J	165	VAL	3.0
4	I	171	ARG	3.0
1	A	217	TRP	3.0
1	A	273	ARG	3.0
5	J	204	ARG	2.9
5	E	219	ASN	2.9
4	I	61	GLU	2.9
4	I	128	TYR	2.9
1	F	224	GLN	2.9
4	I	183	TRP	2.9
1	A	228	THR	2.9
5	J	183	ASN	2.8
4	I	54	TYR	2.8
5	J	161	ASN	2.8
1	A	198	GLU	2.8
5	J	131	GLU	2.8
1	A	192	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	J	198	THR	2.8
5	E	16	LYS	2.8
5	E	143	VAL	2.8
5	J	222	TRP	2.8
4	I	193	ASN	2.8
5	E	148	GLY	2.7
4	D	171	ARG	2.7
5	E	223	THR	2.7
5	E	183	ASN	2.7
5	J	137	THR	2.7
4	D	130	LEU	2.7
5	J	110	LEU	2.7
1	A	227	ASP	2.7
1	A	225	THR	2.6
5	E	116	LEU	2.6
4	D	131	ARG	2.6
5	J	228	LYS	2.6
5	J	112	VAL	2.6
5	E	142	LEU	2.6
1	A	218	GLN	2.6
1	A	189	MET	2.6
1	A	219	ARG	2.5
1	A	266	LEU	2.5
1	F	251	SER	2.5
1	F	138	MET	2.5
1	F	204	TRP	2.5
4	I	137	ASP	2.5
4	I	188	ASP	2.5
1	A	200	THR	2.5
5	J	134	ILE	2.5
4	I	129	GLN	2.4
5	J	136	HIS	2.4
4	I	141	CYS	2.4
5	E	218	GLU	2.4
1	F	272	LEU	2.4
4	D	84	LEU	2.4
4	D	168	LEU	2.4
5	J	124	VAL	2.4
5	E	86	ASN	2.4
5	E	238	ALA	2.4
4	I	143	PHE	2.4
5	E	151	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	2.4
1	F	200	THR	2.4
4	I	84	LEU	2.4
5	J	143	VAL	2.3
1	F	250	PRO	2.3
5	E	120	PHE	2.3
5	E	181	ALA	2.3
4	D	127	VAL	2.3
1	A	197	HIS	2.3
4	I	175	PHE	2.2
4	I	121	GLN	2.2
1	F	225	THR	2.2
5	J	215	GLY	2.2
4	I	146	PHE	2.2
4	I	131	ARG	2.2
5	J	111	THR	2.2
4	D	66	VAL	2.2
4	I	57	GLN	2.2
1	F	190	THR	2.2
2	B	1	ILE	2.2
5	E	193	LEU	2.2
2	G	0	MET	2.2
2	G	75	LYS	2.2
4	D	120	ILE	2.2
2	B	75	LYS	2.1
1	A	193	ALA	2.1
5	J	197	ALA	2.1
5	J	233	ILE	2.1
1	A	204	TRP	2.1
5	J	100	TYR	2.1
5	J	160	VAL	2.1
5	E	156	LEU	2.1
5	J	194	ARG	2.1
1	A	221	GLY	2.1
1	A	226	GLN	2.1
4	D	121	GLN	2.1
1	F	266	LEU	2.1
4	I	168	LEU	2.1
5	E	207	PHE	2.1
5	J	17	GLU	2.1
2	G	19	LYS	2.1
4	I	127	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	251	SER	2.0
2	B	99	MET	2.0
5	J	122	PRO	2.0
4	I	154	GLN	2.0
4	I	195	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	EDT	E	301	20/20	0.73	0.30	3.85	26,36,45,45	32
6	EDT	J	301	20/20	0.74	0.31	3.58	29,37,44,47	32

6.5 Other polymers (i)

There are no such residues in this entry.