



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:27 AM BST

PDB ID : 6VMX  
Title : Structure of HD14 TCR in complex with HLA-B7 presenting an EBV epitope  
Authors : Farenc, C.; Rossjohn, J.; Gras, S.  
Deposited on : 2020-01-28  
Resolution : 3.10 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 : 2.14.6  
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) : 2.14.6

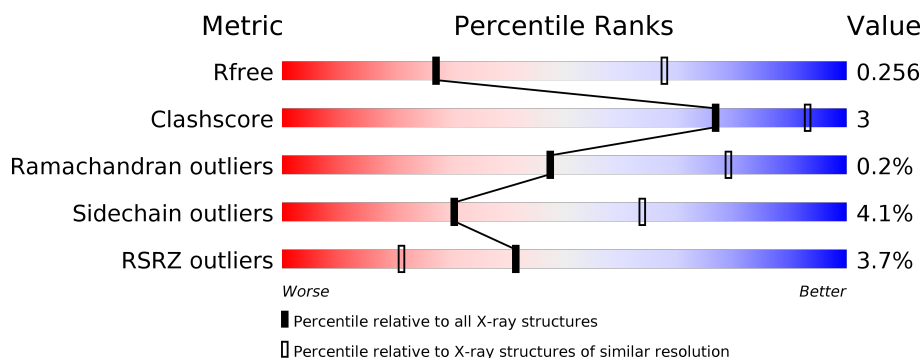
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	276	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
1	F	276	<div> <div>14%</div> <div>84%</div> <div>10%</div> </div>
2	B	100	<div> <div>3%</div> <div>86%</div> <div>13%</div> </div>
2	G	100	<div> <div>%</div> <div>86%</div> <div>14%</div> </div>
3	C	9	<div> <div>78%</div> <div>22%</div> </div>
3	H	9	<div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	203	<div><div>%</div><div><div></div><div>86%</div><div>14%</div></div></div>
4	I	203	<div><div>%</div><div><div></div><div>90%</div><div>10%</div></div></div>
5	E	243	<div><div>2%</div><div><div></div><div>91%</div><div>9%</div></div></div>
5	J	243	<div><div></div><div><div></div><div>92%</div><div>8%</div></div></div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13564 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 HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	3	0
			2287	1417	418	446	6			
1	F	267	Total	C	N	O	S	0	2	0
			2201	1363	403	429	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			845	539	142	160	4			
2	G	100	Total	C	N	O	S	0	1	0
			845	539	142	160	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 Epstein-Barr nuclear antigen 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			83	55	18	10			
3	H	9	Total	C	N	O	0	0	0
			83	55	18	10			

- Molecule 4 is a protein called HD14 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	203	Total	C	N	O	S	0	0	0
			1591	998	260	324	9			

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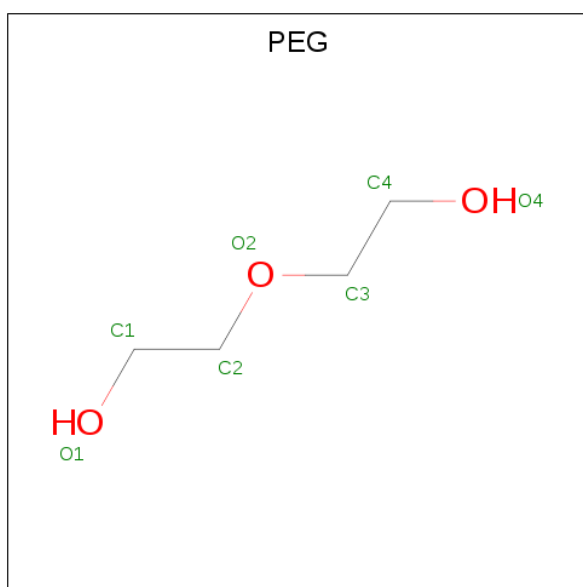
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	203	Total	C	N	O	S	0	0	0
			1591	998	260	324	9			

- Molecule 5 is a protein called HD14 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1943	1228	334	370	11			
5	J	242	Total	C	N	O	S	0	0	0
			1935	1224	333	367	11			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		
6	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		

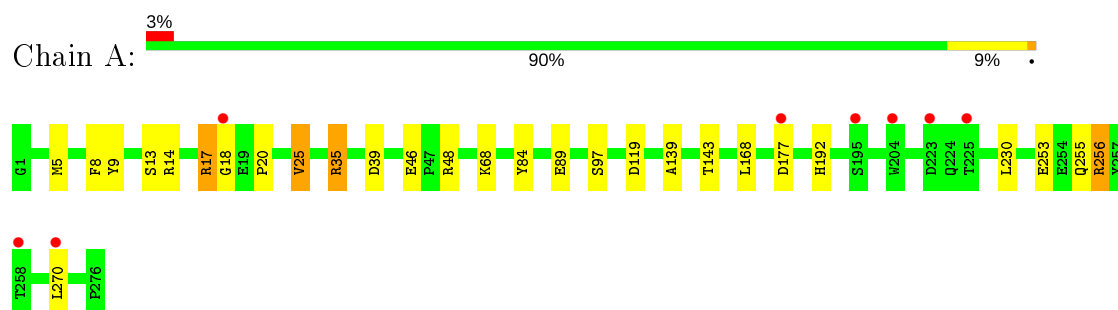
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	17	Total	O	0	0
			17	17		
8	B	5	Total	O	0	0
			5	5		
8	D	9	Total	O	0	0
			9	9		
8	E	33	Total	O	0	0
			33	33		
8	F	19	Total	O	0	0
			19	19		
8	G	5	Total	O	0	0
			5	5		
8	I	17	Total	O	0	0
			17	17		
8	J	22	Total	O	0	0
			22	22		

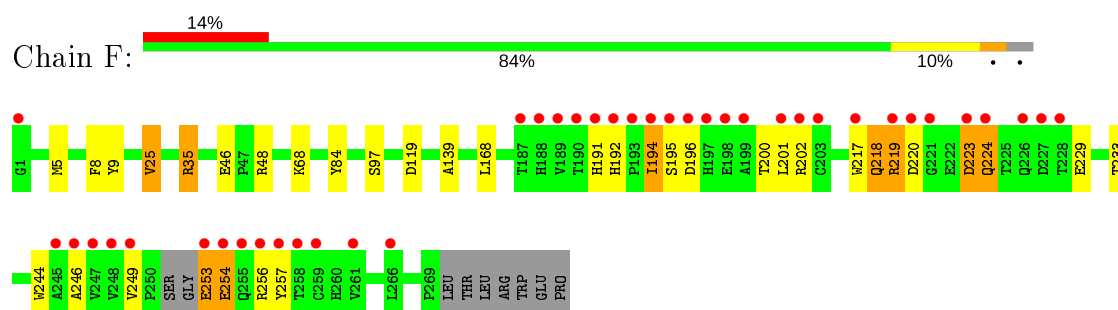
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

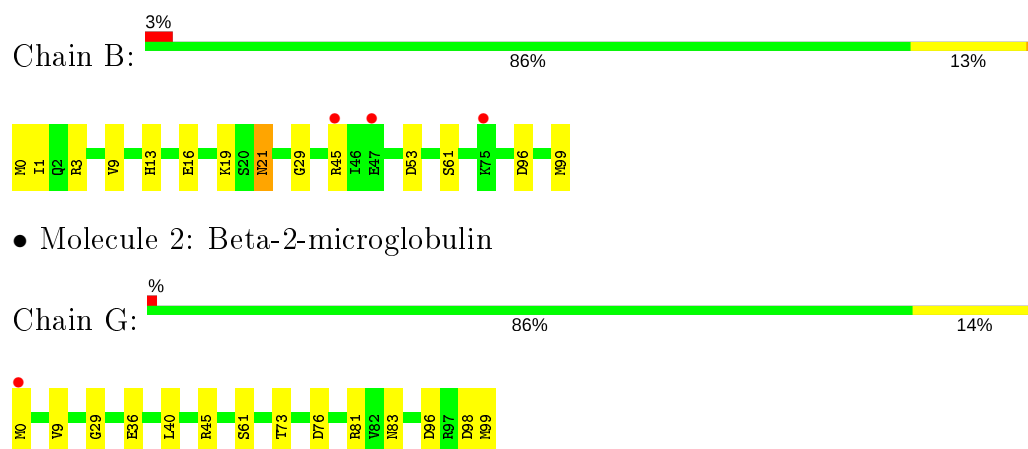
- Molecule 1: HLA class I histocompatibility antigen, B-7 alpha chain




- Molecule 1: HLA class I histocompatibility antigen, B-7 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Epstein-Barr nuclear antigen 3

Chain C:  78% 22%




- Molecule 3: Epstein-Barr nuclear antigen 3

Chain H:  89% 11%




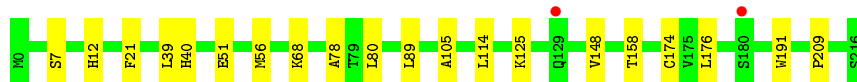
- Molecule 4: HD14 alpha chain

Chain D:  86% 14%




- Molecule 4: HD14 alpha chain

Chain I:  90% 10%



- Molecule 5: HD14 beta chain

Chain E:  91% 9%



- Molecule 5: HD14 beta chain

Chain J:  92% 8%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.46 Å   181.09 Å   190.29 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.71 – 3.10 48.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.71-3.10) 100.0 (48.71-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 3.12 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.221   ,   0.242 0.238   ,   0.256	Depositor DCC
$R_{free}$ test set	2615 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	13564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

### 5.1 Standard geometry

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

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	0.38	0/2350	0.42	0/3192
1	F	0.39	0/2260	0.47	0/3068
2	B	0.38	0/868	0.40	0/1173
2	G	0.40	0/868	0.42	0/1173
3	C	0.46	0/85	0.38	0/112
3	H	0.46	0/85	0.39	0/112
4	D	0.40	0/1628	0.44	0/2205
4	I	0.37	0/1628	0.42	0/2205
5	E	0.37	0/1998	0.42	0/2716
5	J	0.37	0/1990	0.42	0/2705
All	All	0.38	0/13760	0.43	0/18661

There are no bond length outliers.

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	2287	0	2123	11	0
1	F	2201	0	2041	22	0
2	B	845	0	815	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	845	0	813	7	0
3	C	83	0	97	2	0
3	H	83	0	97	1	0
4	D	1591	0	1506	13	0
4	I	1591	0	1506	9	0
5	E	1943	0	1865	10	0
5	J	1935	0	1858	7	0
6	A	7	0	10	0	0
6	F	7	0	10	0	0
6	J	7	0	10	0	0
7	A	4	0	6	0	0
7	E	8	0	12	0	0
8	A	17	0	0	0	0
8	B	5	0	0	0	0
8	D	9	0	0	0	0
8	E	33	0	0	0	0
8	F	19	0	0	0	0
8	G	5	0	0	0	0
8	I	17	0	0	0	0
8	J	22	0	0	0	0
All	All	13564	0	12769	78	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 3.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LEU:HD11	1:F:254:GLU:HB3	1.55	0.86
1:F:201:LEU:HD11	1:F:254:GLU:CB	2.10	0.80
1:F:218:GLN:HG2	1:F:223:ASP:HB3	1.65	0.78
1:F:218:GLN:HA	1:F:223:ASP:HA	1.65	0.78
2:B:16:GLU:OE1	2:B:19:LYS:HD2	1.87	0.74
1:F:202:ARG:NH2	2:G:98:ASP:HB3	2.06	0.71
4:D:176:LEU:HB3	5:E:183:CYS:HB2	1.76	0.67
1:F:219:ARG:HB2	1:F:224:GLN:HB2	1.79	0.64
4:D:138:LEU:HD13	4:D:148:VAL:HG23	1.80	0.64
1:A:253:GLU:HG2	1:A:256:ARG:HD2	1.83	0.61
4:D:126:PRO:HG2	4:D:175:VAL:HG11	1.83	0.60
4:I:158:THR:HG21	4:I:209:PRO:HG3	1.83	0.59
1:F:202:ARG:HG2	1:F:246:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HB3	1:A:17:ARG:HB2	1.86	0.58
4:D:137:GLN:O	5:E:143:SER:HB2	2.03	0.57
1:F:219:ARG:HG3	1:F:257:TYR:CE1	2.38	0.57
4:D:44:TRP:HB3	4:D:101:THR:HG23	1.86	0.56
1:F:9:TYR:HB2	1:F:97:SER:HB2	1.87	0.56
1:A:9:TYR:HB2	1:A:97:SER:HB2	1.87	0.56
5:J:142:PRO:HD3	5:J:155:LEU:HG	1.88	0.56
4:D:148:VAL:HG12	4:D:191:TRP:HB3	1.87	0.55
3:H:5:PHE:HB2	5:J:112:THR:HG23	1.88	0.55
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.72	0.55
5:E:142:PRO:HD3	5:E:155:LEU:HG	1.88	0.55
2:G:96:ASP:HB3	2:G:99:MET:HB2	1.90	0.54
5:J:91:LEU:HD23	5:J:94:LEU:HD11	1.90	0.54
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.90	0.54
5:E:165:ASP:HB2	5:E:188:PRO:HG2	1.90	0.54
5:J:165:ASP:HB2	5:J:188:PRO:HG2	1.89	0.53
1:F:219:ARG:HG3	1:F:257:TYR:CZ	2.43	0.53
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.91	0.53
4:I:40:HIS:HB2	4:I:105:ALA:HB3	1.90	0.53
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.89	0.53
5:E:91:LEU:HD23	5:E:94:LEU:HD11	1.90	0.53
4:D:40:HIS:HB2	4:D:105:ALA:HB3	1.90	0.52
1:A:119:ASP:HB3	2:B:0:MET:HB2	1.92	0.51
2:G:36:GLU:HB2	2:G:83:ASN:HB3	1.94	0.50
1:A:143:THR:HG22	3:C:9:LEU:O	2.12	0.49
4:I:12:HIS:HB3	4:I:125:LYS:HE3	1.94	0.49
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.95	0.48
4:D:78:ALA:HB2	4:D:89:LEU:HD12	1.97	0.47
1:F:8:PHE:HB2	1:F:25:VAL:HG23	1.97	0.47
5:J:39:MET:HB3	5:J:87:LEU:HD22	1.95	0.47
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.97	0.47
5:E:39:MET:HB3	5:E:87:LEU:HD22	1.96	0.46
1:A:8:PHE:HB2	1:A:25:VAL:HG23	1.97	0.46
1:F:84:TYR:HB3	1:F:139:ALA:HB1	1.97	0.46
1:A:35:ARG:HG2	1:A:48:ARG:HD3	1.98	0.46
4:I:176:LEU:HB3	5:J:183:CYS:HB2	1.97	0.46
4:D:101:THR:HA	4:D:121:THR:HA	1.99	0.45
4:I:78:ALA:HB2	4:I:89:LEU:HD12	1.97	0.45
1:A:84:TYR:HB3	1:A:139:ALA:HB1	1.98	0.45
1:F:35:ARG:HG2	1:F:48:ARG:HD3	1.98	0.45
2:G:73:THR:HB	2:G:76:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:ILE:HG13	1:F:200:THR:HG23	1.98	0.44
1:F:217:TRP:O	1:F:218:GLN:HB2	2.18	0.44
4:D:50:PRO:HD2	5:E:117:PHE:HB3	2.00	0.44
3:C:5:PHE:HB2	5:E:112:THR:HG23	2.00	0.44
1:F:119:ASP:HB3	2:G:0:MET:HG3	2.00	0.44
1:F:191:HIS:HA	1:F:201:LEU:HD23	2.00	0.43
5:J:55:VAL:HB	5:J:67:ILE:HB	1.99	0.43
5:E:55:VAL:HB	5:E:67:ILE:HB	2.00	0.43
5:E:44:GLN:HG3	5:E:101:LEU:HB3	2.00	0.42
4:D:105:ALA:HB1	4:D:114:LEU:HD22	2.01	0.42
1:F:194:ILE:HG22	1:F:195:SER:H	1.85	0.42
1:A:35:ARG:HD3	2:B:53:ASP:OD1	2.20	0.41
4:I:148:VAL:HG12	4:I:191:TRP:HB3	2.03	0.41
2:B:3:ARG:HH11	2:B:61:SER:HB3	1.84	0.41
1:F:229:GLU:HB3	1:F:244:TRP:HZ3	1.85	0.41
4:D:75:ARG:HD2	4:D:93:GLY:H	1.85	0.41
1:A:13:SER:HA	1:A:20:PRO:HB3	2.03	0.41
4:I:105:ALA:HB1	4:I:114:LEU:HD22	2.02	0.41
4:I:56:MET:HB3	4:I:80:LEU:HD22	2.03	0.41
4:D:56:MET:HB3	4:D:80:LEU:HD22	2.03	0.40
1:F:220:ASP:OD1	1:F:256:ARG:HB2	2.21	0.40
4:I:114:LEU:HD23	4:I:114:LEU:HA	1.96	0.40
1:F:253:GLU:OE2	1:F:253:GLU:HA	2.21	0.40
2:G:40:LEU:HD11	2:G:81:ARG:HB2	2.04	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	277/276 (100%)	261 (94%)	15 (5%)	1 (0%)	34 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	265/276 (96%)	248 (94%)	15 (6%)	2 (1%)	19	54
2	B	99/100 (99%)	96 (97%)	3 (3%)	0	100	100
2	G	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
4	I	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
5	E	241/243 (99%)	230 (95%)	11 (5%)	0	100	100
5	J	240/243 (99%)	230 (96%)	9 (4%)	1 (0%)	34	69
All	All	1637/1662 (98%)	1551 (95%)	82 (5%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	46	ALA
1	F	196	ASP
1	F	218	GLN
1	A	18	GLY

### 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	237/234 (101%)	224 (94%)	13 (6%)	21	53
1	F	228/234 (97%)	215 (94%)	13 (6%)	20	52
2	B	96/95 (101%)	92 (96%)	4 (4%)	30	62
2	G	96/95 (101%)	94 (98%)	2 (2%)	53	79
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	182/182 (100%)	173 (95%)	9 (5%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	182/182 (100%)	176 (97%)	6 (3%)	38	69
5	E	216/216 (100%)	209 (97%)	7 (3%)	39	69
5	J	215/216 (100%)	209 (97%)	6 (3%)	43	73
All	All	1470/1472 (100%)	1410 (96%)	60 (4%)	30	64

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	25	VAL
1	A	35	ARG
1	A	39	ASP
1	A	46	GLU
1	A	68	LYS
1	A	89	GLU
1	A	177	ASP
1	A	192	HIS
1	A	230	LEU
1	A	255	GLN
1	A	256	ARG
1	A	270	LEU
2	B	1	ILE
2	B	9	VAL
2	B	21	ASN
2	B	45	ARG
4	D	7	SER
4	D	11	LEU
4	D	21	PHE
4	D	39	LEU
4	D	51	GLU
4	D	109	SER
4	D	118	GLN
4	D	130	ASN
4	D	146	LYS
5	E	44	GLN
5	E	75	ARG
5	E	86	LEU
5	E	128	ASP
5	E	205	ARG
5	E	207	ARG
5	E	237	GLN

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Mol	Chain	Res	Type
1	F	25	VAL
1	F	35	ARG
1	F	46	GLU
1	F	68	LYS
1	F	192	HIS
1	F	194	ILE
1	F	219	ARG
1	F	223	ASP
1	F	224	GLN
1	F	233	THR
1	F	249	VAL
1	F	253	GLU
1	F	254	GLU
2	G	9	VAL
2	G	45	ARG
4	I	7	SER
4	I	21	PHE
4	I	39	LEU
4	I	51	GLU
4	I	68	LYS
4	I	174	CYS
5	J	75	ARG
5	J	86	LEU
5	J	128	ASP
5	J	205	ARG
5	J	207	ARG
5	J	237	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
5	E	232	ASN
1	F	218	GLN
1	F	224	GLN
5	J	237	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides 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	$\# Z  > 2$
6	PEG	F	301	-	6,6,6	0.07	0	5,5,5	0.04	0
6	PEG	J	301	-	6,6,6	0.09	0	5,5,5	0.02	0
7	EDO	E	301	-	3,3,3	0.58	0	2,2,2	0.33	0
6	PEG	A	301	-	6,6,6	0.08	0	5,5,5	0.02	0
7	EDO	E	302	-	3,3,3	0.63	0	2,2,2	0.24	0
7	EDO	A	302	-	3,3,3	0.60	0	2,2,2	0.31	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
6	PEG	F	301	-	-	1/4/4/4	-
6	PEG	J	301	-	-	1/4/4/4	-
7	EDO	E	301	-	-	0/1/1/1	-
6	PEG	A	301	-	-	2/4/4/4	-
7	EDO	E	302	-	-	0/1/1/1	-
7	EDO	A	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	PEG	C4-C3-O2-C2
6	F	301	PEG	C1-C2-O2-C3
6	A	301	PEG	C1-C2-O2-C3
6	J	301	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	276/276 (100%)	0.16	8 (2%) 51 28	21, 43, 78, 92	0
1	F	267/276 (96%)	0.42	40 (14%) 2 1	17, 37, 93, 106	10 (3%)
2	B	100/100 (100%)	0.10	3 (3%) 50 27	34, 47, 67, 77	0
2	G	100/100 (100%)	0.05	1 (1%) 82 67	29, 55, 78, 84	0
3	C	9/9 (100%)	-0.48	0 100 100	21, 25, 35, 35	0
3	H	9/9 (100%)	-0.63	0 100 100	17, 17, 31, 31	0
4	D	203/203 (100%)	0.19	2 (0%) 82 67	21, 47, 69, 76	2 (0%)
4	I	203/203 (100%)	0.04	2 (0%) 82 67	12, 38, 58, 74	2 (0%)
5	E	243/243 (100%)	-0.12	4 (1%) 72 51	17, 34, 65, 77	2 (0%)
5	J	242/243 (99%)	-0.14	1 (0%) 92 84	14, 33, 57, 66	2 (0%)
All	All	1652/1662 (99%)	0.09	61 (3%) 41 21	12, 40, 75, 106	18 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	SER	4.6
1	F	195	SER	4.3
1	F	249	VAL	4.2
1	F	254	GLU	4.1
1	F	257	TYR	4.0
1	F	188	HIS	4.0
1	F	246	ALA	3.8
1	F	259	CYS	3.6
1	F	191	HIS	3.6
1	F	227	ASP	3.4
1	F	199	ALA	3.4
1	F	224	GLN	3.4
1	F	196	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	18	GLY	3.2
1	F	255	GLN	3.2
4	I	129	GLN	3.2
1	A	225	THR	3.1
5	E	236	THR	3.1
1	F	258	THR	3.0
1	F	202	ARG	2.9
5	E	256	ASP	2.9
4	D	195	SER	2.8
1	F	201	LEU	2.8
1	A	258	THR	2.8
4	I	180	SER	2.7
1	F	221	GLY	2.7
1	F	228	THR	2.7
1	F	261	VAL	2.6
1	F	220	ASP	2.6
1	F	1	GLY	2.6
1	F	217	TRP	2.5
1	F	226	GLN	2.5
1	F	219	ARG	2.5
1	F	187	THR	2.5
1	F	190	THR	2.4
1	F	203	CYS	2.4
5	J	256	ASP	2.4
1	F	194	ILE	2.4
1	F	247	VAL	2.3
1	F	223	ASP	2.3
1	F	245	ALA	2.3
2	G	0	MET	2.3
1	F	266	LEU	2.3
1	A	177	ASP	2.2
1	F	189	VAL	2.2
1	F	248	VAL	2.2
1	A	223	ASP	2.2
2	B	47	GLU	2.2
1	A	270	LEU	2.2
1	F	256	ARG	2.2
1	F	197	HIS	2.2
1	F	193	PRO	2.2
5	E	1	ASP	2.2
2	B	45	ARG	2.2
1	A	204	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	139	ARG	2.1
5	E	197	ASP	2.1
1	F	192	HIS	2.1
2	B	75	LYS	2.1
1	F	253	GLU	2.1
1	F	198	GLU	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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
7	EDO	E	301	4/4	0.83	0.24	23,24,24,24	0
7	EDO	E	302	4/4	0.83	0.25	26,26,27,27	0
6	PEG	J	301	7/7	0.86	0.32	42,43,45,45	0
6	PEG	A	301	7/7	0.88	0.22	50,50,50,50	0
6	PEG	F	301	7/7	0.93	0.29	29,29,30,30	0
7	EDO	A	302	4/4	0.93	0.24	19,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.