



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:41 am BST

PDB ID : 5WJL  
Title : Crystal Structure of HLA-A\*11:01 with GTS1 peptide  
Authors : Gras, S.; Rossjohn, J.  
Deposited on : 2017-07-23  
Resolution : 3.15 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
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

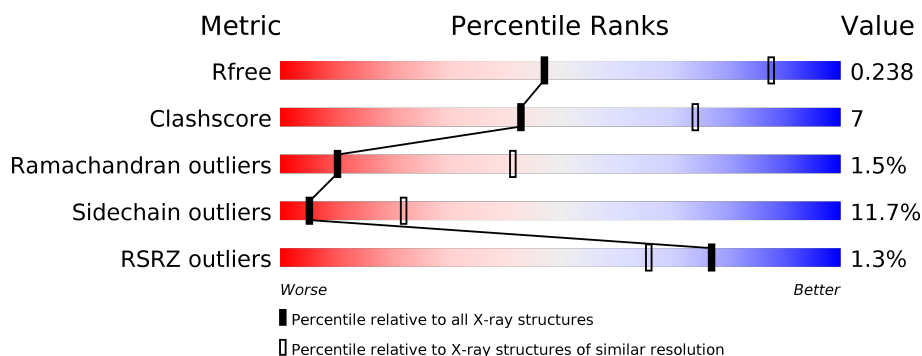
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	274	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
1	D	274	<div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	G	274	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	100	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>
2	E	100	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>.</div> </div> </div>
2	H	100	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	C	10	<div><div></div><div>70%</div><div>20%</div><div>10%</div></div>
3	F	10	<div><div></div><div>70%</div><div>20%</div><div>10%</div></div>
3	I	10	<div><div>10%</div><div>50%</div><div>30%</div><div>10%</div><div>10%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9520 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, A-11 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2236	1389	407	431	9			
1	D	274	Total	C	N	O	S	0	0	0
			2236	1389	407	431	9			
1	G	274	Total	C	N	O	S	0	0	0
			2236	1389	407	431	9			

- 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	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called GTS1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	40	14	15			
3	F	10	Total	C	N	O	0	0	0
			69	40	14	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	0	0	0
			69	40	14	15			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

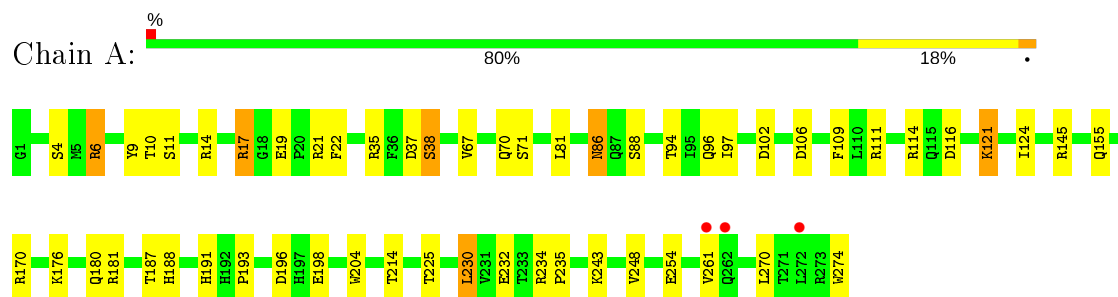
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	7	Total	O	0	0
			7	7		
5	C	2	Total	O	0	0
			2	2		
5	D	28	Total	O	0	0
			28	28		
5	E	6	Total	O	0	0
			6	6		
5	F	3	Total	O	0	0
			3	3		
5	G	20	Total	O	0	0
			20	20		
5	H	4	Total	O	0	0
			4	4		
5	I	1	Total	O	0	0
			1	1		

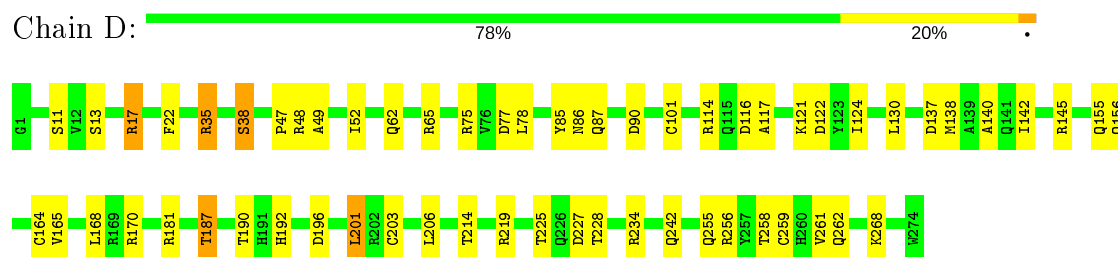
### 3 Residue-property plots [i](#)

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.

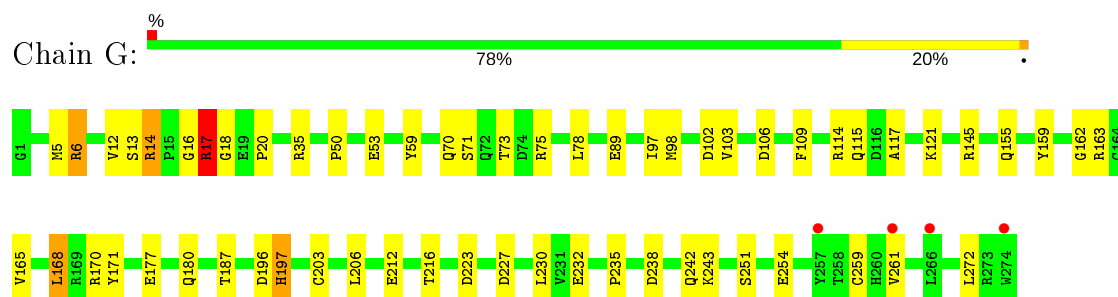
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain



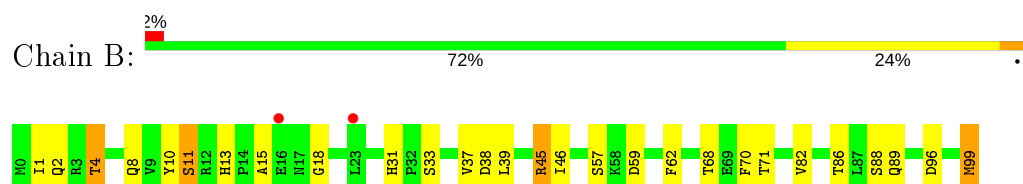
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain



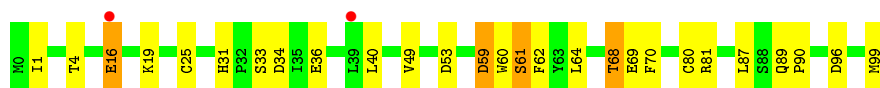
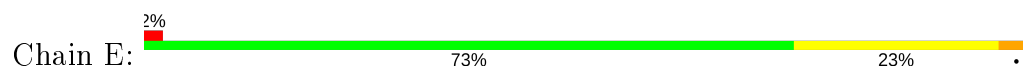
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain



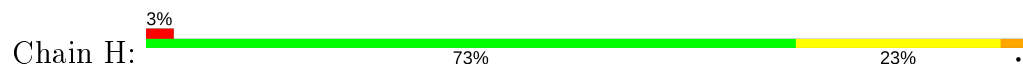
- Molecule 2: Beta-2-microglobulin



## • Molecule 2: Beta-2-microglobulin



## • Molecule 2: Beta-2-microglobulin



## • Molecule 3: GTS1 peptide



## • Molecule 3: GTS1 peptide



## • Molecule 3: GTS1 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.50Å 150.20Å 105.83Å 90.00° 120.53° 90.00°	Depositor
Resolution (Å)	46.90 – 3.15 46.90 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.90-3.15) 99.9 (46.90-3.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.177 , 0.231 0.188 , 0.238	Depositor DCC
$R_{free}$ test set	1815 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 76.1	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	0.94	EDS
Total number of atoms	9520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: CL

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	0.56	0/2297	0.79	0/3117
1	D	0.52	0/2297	0.78	0/3117
1	G	0.52	0/2297	0.79	0/3117
2	B	0.57	0/860	0.84	0/1162
2	E	0.49	0/860	0.80	0/1162
2	H	0.55	0/860	0.80	0/1162
3	C	1.01	0/69	1.17	0/91
3	F	0.71	0/69	1.26	0/91
3	I	0.79	0/69	1.23	0/91
All	All	0.54	0/9678	0.80	0/13110

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	2236	0	2089	21	0
1	D	2236	0	2089	31	0
1	G	2236	0	2089	28	0
2	B	837	0	805	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	837	0	805	13	0
2	H	837	0	804	20	0
3	C	69	0	71	3	0
3	F	69	0	71	3	0
3	I	69	0	71	6	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
5	A	20	0	0	0	0
5	B	7	0	0	0	0
5	C	2	0	0	0	0
5	D	28	0	0	0	0
5	E	6	0	0	0	0
5	F	3	0	0	0	0
5	G	20	0	0	0	0
5	H	4	0	0	1	0
5	I	1	0	0	0	0
All	All	9520	0	8894	116	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 7.

All (116) 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:G:203:CYS:HG	1:G:259:CYS:HG	1.09	0.94
1:D:203:CYS:HG	1:D:259:CYS:HG	0.98	0.86
2:H:33:SER:N	2:H:62:PHE:HE2	1.75	0.84
1:A:155:GLN:HB3	3:C:6:PRO:HD3	1.63	0.79
1:G:155:GLN:HB2	3:I:6:PRO:HD3	1.65	0.77
2:H:33:SER:HA	2:H:62:PHE:CE2	2.21	0.76
1:A:97:ILE:HD11	3:C:10:ARG:HH22	1.49	0.76
2:H:25:CYS:HG	2:H:80:CYS:HG	0.78	0.75
2:E:25:CYS:HG	2:E:80:CYS:HG	0.78	0.75
2:H:33:SER:CA	2:H:62:PHE:CE2	2.70	0.74
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.22	0.74
2:H:33:SER:N	2:H:62:PHE:CE2	2.55	0.74
2:H:21:ASN:HB3	2:H:70:PHE:HE1	1.56	0.70
1:D:155:GLN:HB3	3:F:6:PRO:HD3	1.74	0.69
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.74	0.68
1:D:214:THR:HB	1:D:262:GLN:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:MET:HG3	5:H:103:HOH:O	1.95	0.67
1:D:35:ARG:HG2	1:D:48:ARG:HD2	1.80	0.63
1:D:62:GLN:HE21	1:D:65:ARG:HH11	1.46	0.63
2:H:33:SER:HA	2:H:62:PHE:CD2	2.35	0.62
1:G:235:PRO:HG2	2:H:65:LEU:HD22	1.81	0.61
1:D:101:CYS:HG	1:D:164:CYS:HG	0.61	0.61
1:G:159:TYR:OH	3:I:1:GLY:O	2.16	0.61
1:D:85:TYR:HB2	1:D:87:GLN:HE21	1.67	0.59
1:D:48:ARG:NH1	2:E:53:ASP:OD2	2.29	0.59
2:H:7:ILE:HG12	2:H:82:VAL:HG21	1.86	0.58
1:D:62:GLN:NE2	1:D:65:ARG:HD2	2.19	0.57
1:A:97:ILE:HD11	3:C:10:ARG:NH2	2.19	0.56
1:D:203:CYS:HG	1:D:259:CYS:CB	2.17	0.56
1:G:238:ASP:HB3	2:H:12:ARG:HD3	1.88	0.56
2:B:38:ASP:OD1	2:B:45:ARG:HD3	2.06	0.56
1:D:62:GLN:HE21	1:D:65:ARG:NH1	2.04	0.56
1:G:155:GLN:CB	3:I:6:PRO:HD3	2.35	0.55
1:D:101:CYS:CB	1:D:164:CYS:SG	2.95	0.54
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.41	0.54
1:A:121:LYS:HB2	2:B:1:ILE:HD13	1.90	0.54
1:A:14:ARG:HB2	1:A:17:ARG:HD3	1.89	0.54
1:A:22:PHE:H	1:A:38:SER:HB3	1.73	0.54
1:D:187:THR:HG21	1:D:261:VAL:HG21	1.89	0.54
1:G:206:LEU:HG	1:G:242:GLN:HG2	1.89	0.54
1:D:85:TYR:CB	1:D:87:GLN:HE21	2.21	0.53
1:G:50:PRO:HA	1:G:53:GLU:HG3	1.90	0.53
1:D:22:PHE:H	1:D:38:SER:HB3	1.72	0.53
1:D:62:GLN:NE2	1:D:65:ARG:HH11	2.06	0.53
1:D:101:CYS:HB3	1:D:164:CYS:SG	2.50	0.52
1:G:14:ARG:HB2	1:G:17:ARG:HB2	1.91	0.52
1:G:97:ILE:HD11	3:I:10:ARG:HH22	1.74	0.52
2:E:1:ILE:H	2:E:1:ILE:HD12	1.73	0.52
2:E:40:LEU:HD11	2:E:81:ARG:HB2	1.92	0.52
1:G:16:GLY:C	1:G:18:GLY:H	2.13	0.52
2:E:89:GLN:HG3	2:E:90:PRO:HD2	1.92	0.52
1:G:162:GLY:O	1:G:165:VAL:HG22	2.10	0.51
1:G:203:CYS:CB	1:G:259:CYS:HG	2.22	0.51
2:H:62:PHE:O	2:H:63:TYR:HB3	2.11	0.51
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.93	0.50
1:G:70:GLN:HA	3:I:7:ILE:HD11	1.92	0.50
2:E:16:GLU:HB3	2:E:19:LYS:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:96:ASP:HB3	2:E:99:MET:HB2	1.92	0.50
1:D:234:ARG:HG2	1:D:242:GLN:HB2	1.94	0.49
1:G:235:PRO:CG	2:H:65:LEU:HD22	2.42	0.49
2:H:27:VAL:HG21	2:H:37:VAL:HG21	1.93	0.49
1:G:20:PRO:HD2	1:G:75:ARG:HD2	1.93	0.49
1:G:97:ILE:HD11	3:I:10:ARG:NH2	2.27	0.49
2:H:63:TYR:C	2:H:63:TYR:CD1	2.85	0.49
2:B:11:SER:HB2	2:B:13:HIS:O	2.12	0.48
1:A:21:ARG:HH21	1:A:37:ASP:CG	2.16	0.48
1:D:206:LEU:HG	1:D:242:GLN:HG2	1.96	0.48
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.48
1:G:230:LEU:HD22	1:G:243:LYS:HE3	1.96	0.47
1:A:176:LYS:HA	1:A:180:GLN:HG3	1.96	0.47
1:G:59:TYR:HH	1:G:171:TYR:HH	1.60	0.47
1:G:13:SER:HB3	1:G:78:LEU:HD13	1.97	0.46
1:D:137:ASP:H	1:D:140:ALA:HB3	1.80	0.46
1:G:6:ARG:NH2	1:G:102:ASP:OD1	2.49	0.46
2:E:49:VAL:HG22	2:E:68:THR:HB	1.97	0.46
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.98	0.46
1:A:9:TYR:CD2	1:A:70:GLN:HG2	2.51	0.46
1:A:234:ARG:HD3	2:B:8:GLN:OE1	2.15	0.46
1:G:5:MET:HB2	1:G:168:LEU:HG	1.97	0.46
2:B:8:GLN:O	2:B:10:TYR:CD1	2.69	0.45
1:G:103:VAL:HG22	1:G:168:LEU:HD13	1.98	0.45
2:B:31:HIS:CD2	2:B:62:PHE:CE2	3.05	0.45
1:A:10:THR:HG23	1:A:96:GLN:HG2	1.98	0.45
1:D:47:PRO:HB3	1:D:52:ILE:HG23	1.99	0.45
1:A:188:HIS:CE1	1:A:204:TRP:HB2	2.52	0.45
1:G:187:THR:HG21	1:G:261:VAL:HG21	1.98	0.45
2:H:63:TYR:O	2:H:63:TYR:CD1	2.70	0.45
2:B:57:SER:HB2	2:B:59:ASP:HB3	1.99	0.44
2:E:31:HIS:CD2	2:E:62:PHE:CE2	3.05	0.44
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.85	0.44
1:A:191:HIS:CE1	1:A:193:PRO:HD3	2.52	0.43
1:A:230:LEU:HD22	1:A:243:LYS:HE2	1.99	0.43
1:D:77:ASP:OD2	3:F:10:ARG:NH1	2.51	0.43
1:A:116:ASP:HB2	1:A:124:ILE:HG22	1.99	0.43
2:E:87:LEU:O	4:E:101:CL:CL	2.73	0.43
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.53	0.43
1:D:138:MET:O	1:D:142:ILE:HD12	2.18	0.42
1:A:191:HIS:HB3	1:A:274:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ARG:NH1	1:D:116:ASP:OD1	2.52	0.42
1:A:121:LYS:HB2	2:B:1:ILE:CD1	2.49	0.42
2:B:4:THR:HG23	2:B:86:THR:HB	2.01	0.42
1:D:116:ASP:HB2	1:D:124:ILE:HG22	2.01	0.42
1:D:201:LEU:HA	1:D:201:LEU:HD12	1.91	0.41
1:D:49:ALA:O	1:D:52:ILE:HG22	2.21	0.41
1:G:12:VAL:HG11	2:H:33:SER:HB3	2.01	0.41
1:A:235:PRO:HD2	2:B:10:TYR:OH	2.20	0.41
2:H:37:VAL:HG22	2:H:82:VAL:HG22	2.00	0.41
2:E:25:CYS:CB	2:E:80:CYS:HG	2.27	0.41
2:H:42:ASN:OD1	2:H:77:GLU:N	2.48	0.41
2:B:39:LEU:HB3	2:B:46:ILE:HD12	2.02	0.41
1:D:255:GLN:HE21	1:D:256:ARG:HG3	1.85	0.41
1:A:10:THR:HG21	2:B:62:PHE:CE1	2.56	0.41
1:D:155:GLN:HB3	3:F:6:PRO:CD	2.46	0.41
2:E:59:ASP:HB3	2:E:61:SER:OG	2.21	0.41
1:G:197:HIS:HA	1:G:251:SER:HB2	2.02	0.40
1:D:190:THR:HB	1:D:192:HIS:CE1	2.57	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	272/274 (99%)	252 (93%)	18 (7%)	2 (1%)	22	59
1	D	272/274 (99%)	253 (93%)	18 (7%)	1 (0%)	34	68
1	G	272/274 (99%)	245 (90%)	24 (9%)	3 (1%)	14	48
2	B	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	7	34
2	E	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
2	H	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	1
3	F	8/10 (80%)	6 (75%)	0	2 (25%)	0	0
3	I	8/10 (80%)	5 (62%)	1 (12%)	2 (25%)	0	0
All	All	1134/1152 (98%)	1025 (90%)	92 (8%)	17 (2%)	10	41

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	PRO
3	F	6	PRO
2	H	98	ASP
3	I	6	PRO
1	A	109	PHE
2	B	15	ALA
1	D	17	ARG
1	G	17	ARG
1	G	109	PHE
2	H	29	GLY
1	A	86	ASN
2	H	31	HIS
2	H	62	PHE
2	B	18	GLY
1	G	227	ASP
3	I	7	ILE
3	F	7	ILE

### 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	231/231 (100%)	202 (87%)	29 (13%)	4	19
1	D	231/231 (100%)	204 (88%)	27 (12%)	5	22
1	G	231/231 (100%)	206 (89%)	25 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	95/95 (100%)	84 (88%)	11 (12%)	5	22
2	E	95/95 (100%)	84 (88%)	11 (12%)	5	22
2	H	95/95 (100%)	84 (88%)	11 (12%)	5	22
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	19
3	F	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	6 (75%)	2 (25%)	0	2
All	All	1002/1002 (100%)	885 (88%)	117 (12%)	5	22

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	ARG
1	A	11	SER
1	A	17	ARG
1	A	19	GLU
1	A	35	ARG
1	A	38	SER
1	A	67	VAL
1	A	71	SER
1	A	81	LEU
1	A	86	ASN
1	A	88	SER
1	A	94	THR
1	A	106	ASP
1	A	111	ARG
1	A	114	ARG
1	A	121	LYS
1	A	145	ARG
1	A	170	ARG
1	A	181	ARG
1	A	196	ASP
1	A	198	GLU
1	A	214	THR
1	A	225	THR
1	A	230	LEU
1	A	232	GLU
1	A	248	VAL
1	A	254	GLU
1	A	270	LEU

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Mol	Chain	Res	Type
2	B	2	GLN
2	B	4	THR
2	B	11	SER
2	B	33	SER
2	B	45	ARG
2	B	68	THR
2	B	70	PHE
2	B	71	THR
2	B	88	SER
2	B	89	GLN
2	B	99	MET
3	C	7	ILE
1	D	11	SER
1	D	13	SER
1	D	17	ARG
1	D	35	ARG
1	D	38	SER
1	D	75	ARG
1	D	78	LEU
1	D	86	ASN
1	D	90	ASP
1	D	121	LYS
1	D	122	ASP
1	D	130	LEU
1	D	145	ARG
1	D	156	GLN
1	D	165	VAL
1	D	168	LEU
1	D	170	ARG
1	D	181	ARG
1	D	187	THR
1	D	196	ASP
1	D	201	LEU
1	D	219	ARG
1	D	225	THR
1	D	227	ASP
1	D	228	THR
1	D	258	THR
1	D	268	LYS
2	E	4	THR
2	E	16	GLU
2	E	33	SER

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Mol	Chain	Res	Type
2	E	34	ASP
2	E	36	GLU
2	E	59	ASP
2	E	61	SER
2	E	64	LEU
2	E	68	THR
2	E	69	GLU
2	E	70	PHE
1	G	6	ARG
1	G	14	ARG
1	G	17	ARG
1	G	35	ARG
1	G	71	SER
1	G	73	THR
1	G	89	GLU
1	G	106	ASP
1	G	114	ARG
1	G	115	GLN
1	G	121	LYS
1	G	145	ARG
1	G	163	ARG
1	G	168	LEU
1	G	170	ARG
1	G	177	GLU
1	G	180	GLN
1	G	196	ASP
1	G	197	HIS
1	G	212	GLU
1	G	216	THR
1	G	223	ASP
1	G	232	GLU
1	G	254	GLU
1	G	272	LEU
2	H	0	MET
2	H	2	GLN
2	H	4	THR
2	H	16	GLU
2	H	33	SER
2	H	35	ILE
2	H	61	SER
2	H	63	TYR
2	H	70	PHE

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Mol	Chain	Res	Type
2	H	73	THR
2	H	89	GLN
3	I	3	SER
3	I	7	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	31	HIS
2	B	42	ASN
1	D	62	GLN
1	D	72	GLN
1	D	86	ASN
1	D	87	GLN
1	D	93	HIS
1	D	141	GLN
1	D	156	GLN
1	D	255	GLN
2	E	31	HIS
1	G	72	GLN
1	G	180	GLN

### 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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	274/274 (100%)	-0.08	3 (1%) 80 70	46, 80, 132, 152	0
1	D	274/274 (100%)	-0.14	0 100 100	55, 86, 121, 148	0
1	G	274/274 (100%)	0.08	4 (1%) 73 61	55, 92, 142, 173	0
2	B	100/100 (100%)	0.11	2 (2%) 65 50	57, 98, 137, 147	0
2	E	100/100 (100%)	0.26	2 (2%) 65 50	73, 105, 132, 145	0
2	H	100/100 (100%)	0.34	3 (3%) 50 33	72, 108, 143, 161	0
3	C	10/10 (100%)	0.05	0 100 100	50, 62, 80, 85	0
3	F	10/10 (100%)	-0.02	0 100 100	58, 84, 99, 103	0
3	I	10/10 (100%)	0.58	1 (10%) 7 4	56, 78, 103, 109	0
All	All	1152/1152 (100%)	0.03	15 (1%) 77 66	46, 91, 135, 173	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	6	PRO	4.1
2	H	75	LYS	3.2
1	G	257	TYR	3.1
1	A	262	GLN	2.9
2	E	39	LEU	2.8
2	H	43	GLY	2.6
1	A	261	VAL	2.6
1	G	261	VAL	2.4
1	G	274	TRP	2.4
2	E	16	GLU	2.4
2	H	74	GLU	2.2
2	B	23	LEU	2.2
2	B	16	GLU	2.1
1	G	266	LEU	2.0
1	A	272	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( $\text{\AA}^2$ )	Q<0.9
4	CL	E	101	1/1	0.82	0.23	117,117,117,117	0
4	CL	D	301	1/1	0.90	0.13	90,90,90,90	0
4	CL	C	101	1/1	0.99	0.12	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.