



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 11:15 PM JST

PDB ID : 6K60  
Title : Structural and functional basis for HLA-G isoform recognition of immune checkpoint receptor LILRBs  
Authors : Kuroki, K.; Matsubara, H.; Kanda, R.; Miyashita, N.; Shiroishi, M.; Fukunaga, Y.; Kamishikiryo, J.; Fukunaga, A.; Hirose, K.; Sugita, Y.; Kita, S.; Ose, T.; Maenaka, K.  
Deposited on : 2019-05-31  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

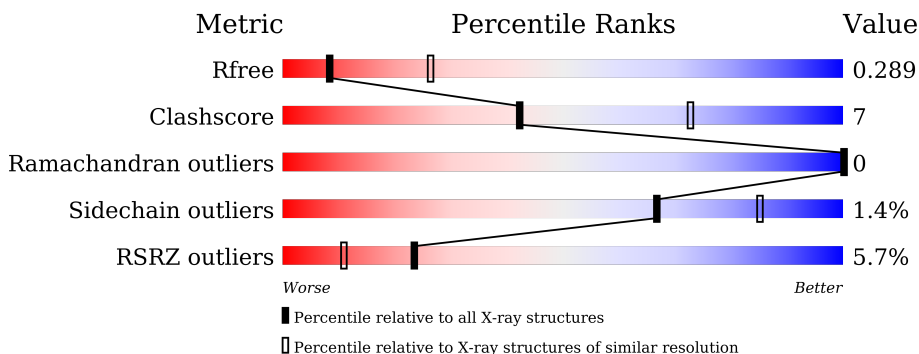
# 1 Overall quality at a glance

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.



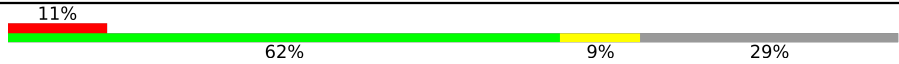

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 of 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	277	 3% 79% 13% 7%
1	E	277	 2% 84% 13% ..
2	B	100	 % 87% 13%
2	F	100	 % 84% 16%
3	C	9	 56% 44%
3	G	9	 89% 11%

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Mol	Chain	Length	Quality of chain
4	D	198	
4	H	198	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7982 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, alpha chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	Total 2092	C 1311	N 374	O 395	S 12	0	0	0
1	E	274	Total 2230	C 1391	N 400	O 427	S 12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P17693
A	42	SER	CYS	engineered mutation	UNP P17693
E	0	MET	-	initiating methionine	UNP P17693
E	42	SER	CYS	engineered mutation	UNP P17693

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	F	100	Total 837	C 533	N 141	O 159	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Peptide from Histone H2A.J.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	Total 81	C 52	N 18	O 11	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	9	Total	C	N	O	0	0	0
			81	52	18	11			

- Molecule 4 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1141	729	193	213	6			
4	H	83	Total	C	N	O	S	0	0	0
			675	438	110	124	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP A0A0G2JQ44
H	0	MET	-	initiating methionine	UNP A0A0G2JQ44

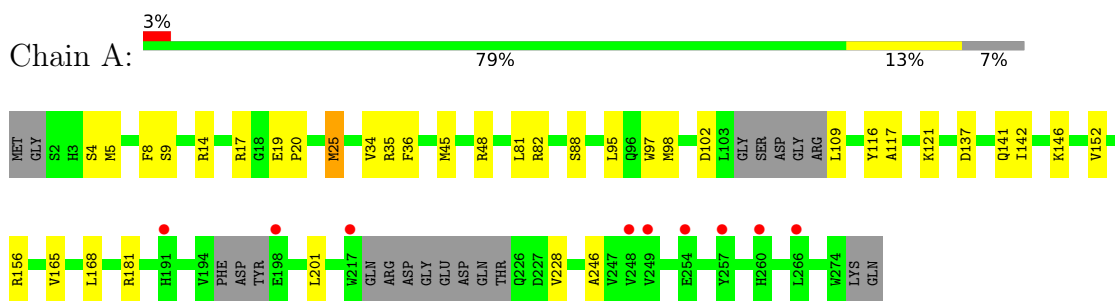
- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	I	0	0
			2	2		
5	B	1	Total	I	0	0
			1	1		
5	C	1	Total	I	0	0
			1	1		
5	E	3	Total	I	0	0
			3	3		
5	G	1	Total	I	0	0
			1	1		

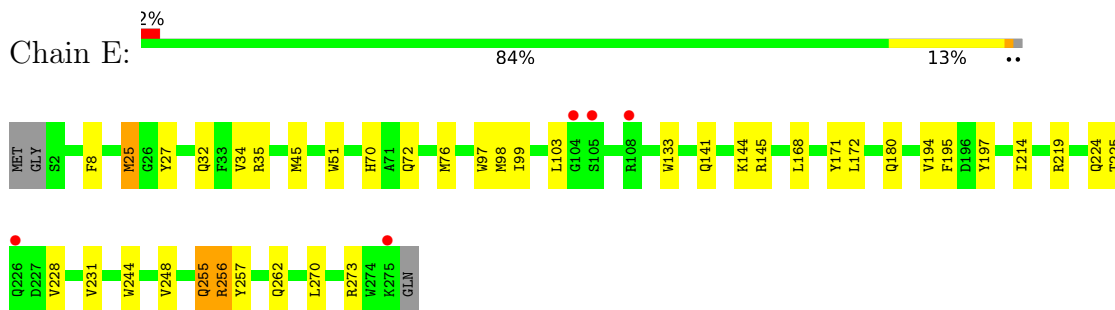
### 3 Residue-property plots [i](#)

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.

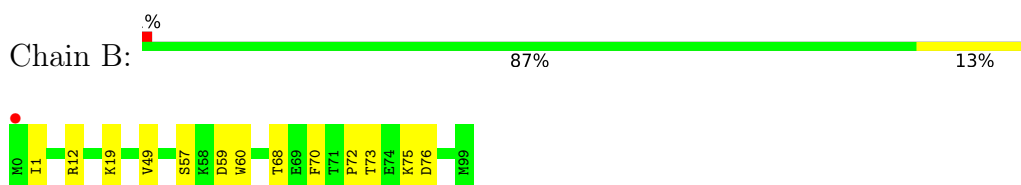
- Molecule 1: HLA class I histocompatibility antigen, alpha chain G



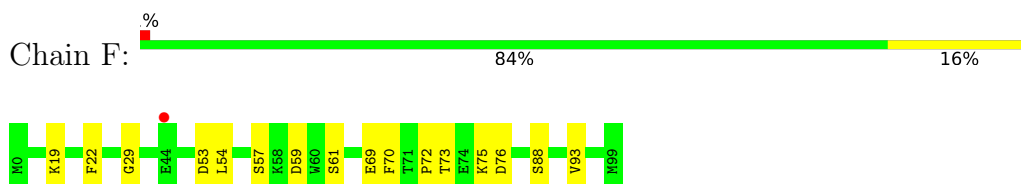
- Molecule 1: HLA class I histocompatibility antigen, alpha chain G



- Molecule 2: Beta-2-microglobulin

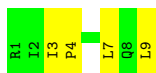


- Molecule 2: Beta-2-microglobulin




- Molecule 3: Peptide from Histone H2A.J

Chain C:  56% 44%



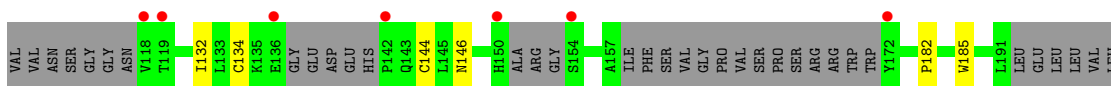
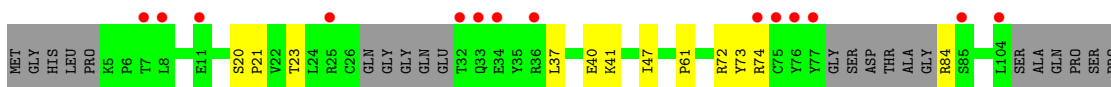
- Molecule 3: Peptide from Histone H2A.J

Chain G:  89% 11%




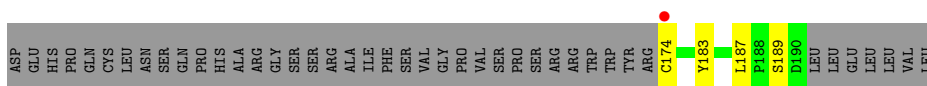
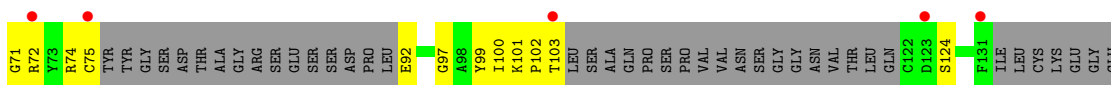
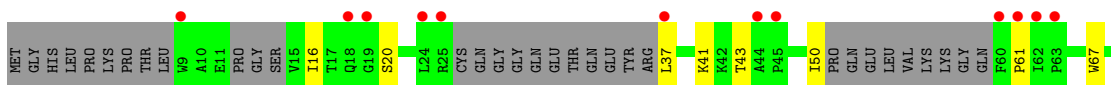
- Molecule 4: Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain D:  11% 62% 9% 29%



- Molecule 4: Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain H:  9% 30% 12% 58%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.38Å 164.38Å 326.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.81 – 3.15 32.81 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.81-3.15) 99.4 (32.81-3.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.261 , 0.289 0.261 , 0.289	Depositor DCC
$R_{free}$ test set	1504 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.0	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.37	0/2148	0.64	0/2915
1	E	0.33	0/2291	0.63	0/3110
2	B	0.32	0/860	0.66	0/1162
2	F	0.35	0/860	0.64	0/1162
3	C	0.35	0/82	0.48	0/108
3	G	0.33	0/82	0.54	0/108
4	D	0.27	0/1170	0.48	0/1586
4	H	0.27	0/693	0.49	0/940
All	All	0.33	0/8186	0.61	0/11091

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2092	0	1964	31	0
1	E	2230	0	2083	33	0
2	B	837	0	803	7	0
2	F	837	0	803	13	0
3	C	81	0	94	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	81	0	94	1	0
4	D	1141	0	1103	9	0
4	H	675	0	636	23	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
All	All	7982	0	7580	107	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 (107) 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:H:100:ILE:HA	4:H:187:LEU:HD12	1.60	0.84
2:F:88:SER:HB3	4:H:187:LEU:HD11	1.69	0.73
1:E:98:MET:HG2	1:E:99:ILE:N	2.06	0.70
1:E:219:ARG:HH11	1:E:256:ARG:NH1	1.89	0.70
2:B:73:THR:HG22	2:B:75:LYS:H	1.58	0.69
1:A:4:SER:HB3	1:A:102:ASP:OD1	1.93	0.67
2:F:73:THR:HG22	2:F:75:LYS:H	1.60	0.67
4:H:102:PRO:HB3	4:H:124:SER:HB2	1.80	0.64
4:H:102:PRO:HB3	4:H:124:SER:CB	2.28	0.64
4:H:102:PRO:HB3	4:H:124:SER:CA	2.27	0.63
1:A:34:VAL:HG22	1:A:45:MET:HG3	1.81	0.63
4:H:102:PRO:HB3	4:H:124:SER:HA	1.79	0.63
1:E:72:GLN:O	1:E:76:MET:HG2	2.00	0.61
1:E:225:THR:HG22	1:E:225:THR:O	2.01	0.60
1:E:256:ARG:HG2	1:E:257:TYR:CD1	2.37	0.60
1:E:172:LEU:HB3	1:E:180:GLN:HE21	1.67	0.59
1:E:219:ARG:HH11	1:E:256:ARG:HH11	1.51	0.57
1:E:194:VAL:HG22	4:H:43:THR:HB	1.86	0.56
1:A:116:TYR:HE2	3:C:7:LEU:HD12	1.71	0.56
1:E:219:ARG:HB3	1:E:224:GLN:HE21	1.70	0.56
1:A:81:LEU:HD11	3:C:9:LEU:HD12	1.88	0.56
4:H:99:TYR:O	4:H:187:LEU:N	2.38	0.56
1:A:35:ARG:HG2	1:A:48:ARG:NH2	2.22	0.54
1:A:82:ARG:HD2	1:A:88:SER:O	2.08	0.53
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:TRP:HB2	1:E:144:LYS:HG3	1.91	0.53
1:E:214:ILE:HB	1:E:262:GLN:HB2	1.91	0.53
1:E:195:PHE:CE2	1:E:197:TYR:HB2	2.44	0.52
2:F:73:THR:HB	2:F:76:ASP:HB2	1.91	0.51
1:E:34:VAL:CG2	1:E:45:MET:HG3	2.40	0.51
4:D:20:SER:OG	4:D:21:PRO:HD2	2.10	0.51
4:D:47:ILE:HD11	4:D:73:TYR:HE2	1.76	0.50
1:E:98:MET:CG	1:E:99:ILE:N	2.75	0.50
1:E:255:GLN:HG3	1:E:273:ARG:HD3	1.93	0.50
1:A:34:VAL:CG2	1:A:45:MET:HG3	2.41	0.50
1:A:142:ILE:O	1:A:146:LYS:HG3	2.12	0.50
2:F:88:SER:CB	4:H:187:LEU:HD11	2.40	0.50
2:F:93:VAL:HG13	4:H:67:TRP:CZ2	2.47	0.49
1:A:81:LEU:HD11	3:C:9:LEU:CD1	2.42	0.49
1:A:137:ASP:O	1:A:141:GLN:HG3	2.13	0.48
1:A:4:SER:CB	1:A:102:ASP:OD1	2.59	0.48
1:A:8:PHE:HE1	1:A:98:MET:SD	2.36	0.48
4:D:40:GLU:O	4:D:41:LYS:CB	2.62	0.48
1:E:224:GLN:O	1:E:228:VAL:HG21	2.14	0.48
4:H:97:GLY:HA2	4:H:187:LEU:HD23	1.96	0.48
1:A:228:VAL:HG13	1:A:246:ALA:O	2.14	0.47
2:B:19:LYS:O	2:B:72:PRO:HD2	2.14	0.47
1:A:116:TYR:CE2	3:C:7:LEU:HD12	2.49	0.47
1:A:121:LYS:HE3	2:B:1:ILE:HG12	1.96	0.47
1:A:35:ARG:HG2	1:A:48:ARG:CZ	2.44	0.47
1:E:34:VAL:HG22	1:E:45:MET:HG3	1.97	0.47
1:A:8:PHE:HB2	1:A:25:MET:SD	2.55	0.47
1:A:181:ARG:NH1	2:F:19:LYS:HD3	2.30	0.47
4:H:100:ILE:HA	4:H:187:LEU:CD1	2.40	0.46
1:A:14:ARG:HB2	1:A:17:ARG:HB2	1.98	0.46
1:A:81:LEU:HD22	1:A:95:LEU:HD13	1.98	0.46
1:E:35:ARG:NH2	2:F:54:LEU:O	2.43	0.46
1:E:70:HIS:ND1	3:G:6:HIS:HD2	2.14	0.46
4:H:99:TYR:O	4:H:187:LEU:HG	2.16	0.46
1:A:109:LEU:HB2	1:A:165:VAL:HG21	1.98	0.45
4:D:23:THR:HA	4:D:61:PRO:HA	1.98	0.45
4:D:37:LEU:HD12	4:D:74:ARG:O	2.15	0.45
4:H:43:THR:O	4:H:43:THR:HG23	2.16	0.45
4:H:102:PRO:CB	4:H:124:SER:HA	2.46	0.45
2:B:73:THR:HB	2:B:76:ASP:HB2	1.99	0.45
4:H:174:CYS:N	4:H:189:SER:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:50:ILE:HD12	4:H:61:PRO:HD2	1.99	0.45
1:E:97:TRP:CH2	1:E:99:ILE:CG2	3.00	0.44
1:E:255:GLN:HA	1:E:255:GLN:OE1	2.16	0.44
4:H:71:GLY:HA2	4:H:183:TYR:CD2	2.53	0.44
1:A:48:ARG:HA	1:A:48:ARG:HD3	1.82	0.44
1:A:201:LEU:O	1:A:246:ALA:HA	2.17	0.44
4:D:134:CYS:HA	4:D:144:CYS:HA	1.97	0.44
4:D:182:PRO:O	4:D:185:TRP:NE1	2.45	0.44
4:H:37:LEU:N	4:H:75:CYS:HG	2.15	0.44
1:E:248:VAL:HG21	4:H:41:LYS:HA	2.00	0.44
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.83	0.43
3:C:3:ILE:HG13	3:C:4:PRO:HD2	2.00	0.43
1:E:25:MET:SD	1:E:25:MET:N	2.90	0.43
2:F:19:LYS:O	2:F:72:PRO:HD2	2.17	0.43
4:H:72:ARG:HG3	4:H:92:GLU:HG2	1.99	0.43
2:B:57:SER:C	2:B:59:ASP:H	2.22	0.43
1:E:141:GLN:O	1:E:145:ARG:HG3	2.18	0.42
1:E:8:PHE:HB2	1:E:25:MET:SD	2.58	0.42
2:F:57:SER:HB3	2:F:59:ASP:OD1	2.20	0.42
1:A:36:PHE:HB2	1:A:45:MET:SD	2.60	0.42
1:E:97:TRP:CH2	1:E:99:ILE:HG21	2.55	0.42
2:F:22:PHE:CE1	2:F:69:GLU:HG2	2.54	0.42
4:D:40:GLU:OE2	4:D:72:ARG:HD3	2.20	0.42
4:H:16:ILE:HG23	4:H:20:SER:HB2	2.01	0.42
1:A:25:MET:SD	1:A:25:MET:N	2.93	0.42
4:D:132:ILE:HD13	4:D:146:ASN:HA	2.02	0.42
1:E:103:LEU:HD13	1:E:168:LEU:HD23	2.02	0.41
1:A:152:VAL:O	1:A:156:ARG:HG2	2.19	0.41
2:F:29:GLY:HA2	2:F:61:SER:HB2	2.01	0.41
1:A:9:SER:OG	1:A:97:TRP:HB3	2.20	0.41
1:E:97:TRP:CZ2	1:E:99:ILE:CG2	3.03	0.41
1:E:35:ARG:CZ	2:F:53:ASP:HB3	2.50	0.41
1:E:231:VAL:HG11	1:E:244:TRP:CZ2	2.56	0.41
1:E:27:TYR:CE2	1:E:32:GLN:HB2	2.56	0.41
1:E:51:TRP:CZ3	1:E:171:TYR:HB3	2.56	0.41
2:F:57:SER:C	2:F:59:ASP:H	2.23	0.41
2:B:49:VAL:HG12	2:B:68:THR:HB	2.03	0.41
1:E:256:ARG:HG2	1:E:257:TYR:CE1	2.55	0.40
4:H:101:LYS:H	4:H:101:LYS:HG3	1.68	0.40
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.03	0.40
1:A:117:ALA:HB2	2:B:60:TRP:CE2	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	249/277 (90%)	241 (97%)	8 (3%)	0	100	100
1	E	272/277 (98%)	264 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	F	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	G	7/9 (78%)	7 (100%)	0	0	100	100
4	D	127/198 (64%)	116 (91%)	11 (9%)	0	100	100
4	H	69/198 (35%)	64 (93%)	5 (7%)	0	100	100
All	All	927/1168 (79%)	891 (96%)	36 (4%)	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	217/233 (93%)	216 (100%)	1 (0%)	88	95
1	E	231/233 (99%)	227 (98%)	4 (2%)	60	82
2	B	95/95 (100%)	93 (98%)	2 (2%)	53	78
2	F	95/95 (100%)	94 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	9/9 (100%)	9 (100%)	0	100	100
3	G	9/9 (100%)	8 (89%)	1 (11%)	6	23
4	D	128/172 (74%)	127 (99%)	1 (1%)	81	92
4	H	73/172 (42%)	71 (97%)	2 (3%)	44	72
All	All	857/1018 (84%)	845 (99%)	12 (1%)	67	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
2	B	12	ARG
2	B	70	PHE
4	D	84	ARG
1	E	25	MET
1	E	255	GLN
1	E	256	ARG
1	E	270	LEU
2	F	70	PHE
3	G	6	HIS
4	H	74	ARG
4	H	103	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	180	GLN
3	G	6	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	257/277 (92%)	0.36	9 (3%) 44 23	49, 77, 117, 131	0
1	E	274/277 (98%)	0.11	5 (1%) 68 49	49, 67, 97, 114	0
2	B	100/100 (100%)	0.04	1 (1%) 82 70	52, 61, 82, 89	0
2	F	100/100 (100%)	0.16	1 (1%) 82 70	52, 70, 91, 102	0
3	C	9/9 (100%)	0.21	0 100 100	56, 61, 72, 76	0
3	G	9/9 (100%)	-0.14	0 100 100	56, 58, 65, 65	0
4	D	141/198 (71%)	0.78	21 (14%) 2 1	65, 86, 110, 125	0
4	H	83/198 (41%)	1.03	18 (21%) 0 0	86, 107, 133, 149	0
All	All	973/1168 (83%)	0.35	55 (5%) 23 11	49, 74, 112, 149	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	150	HIS	4.7
4	H	75	CYS	4.3
4	D	118	VAL	4.2
4	H	45	PRO	4.0
4	H	60	PHE	3.9
4	D	172	TYR	3.9
4	D	154	SER	3.9
1	E	105	SER	3.9
4	D	119	THR	3.8
4	H	37	LEU	3.8
2	B	0	MET	3.3
4	D	74	ARG	3.3
4	H	131	PHE	3.3
1	E	104	GLY	3.2
4	H	103	THR	3.2
4	D	104	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	7	THR	3.0
1	A	248	VAL	3.0
4	D	85	SER	2.9
4	D	76	TYR	2.9
4	H	44	ALA	2.8
4	H	25	ARG	2.8
4	D	33	GLN	2.8
4	H	62	ILE	2.8
1	A	266	LEU	2.6
4	H	9	TRP	2.6
4	D	142	PRO	2.6
4	H	123	ASP	2.5
1	A	260	HIS	2.5
4	D	77	TYR	2.5
4	H	18	GLN	2.5
4	H	19	GLY	2.5
1	E	226	GLN	2.5
1	A	249	VAL	2.4
4	D	8	LEU	2.4
4	H	24	LEU	2.3
1	A	257	TYR	2.3
4	D	136	GLU	2.3
1	A	217	TRP	2.3
2	F	44	GLU	2.2
4	H	61	PRO	2.2
1	A	191	HIS	2.2
4	D	75	CYS	2.2
4	D	11	GLU	2.2
4	D	25	ARG	2.2
4	D	34	GLU	2.2
4	D	32	THR	2.2
4	H	63	PRO	2.1
4	H	72	ARG	2.1
1	E	275	LYS	2.1
1	A	198	GLU	2.1
1	A	254	GLU	2.1
4	H	174	CYS	2.1
4	D	36	ARG	2.0
1	E	108	ARG	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
5	IOD	B	1000	1/1	0.96	0.09	120,120,120,120	0
5	IOD	E	302	1/1	0.96	0.10	86,86,86,86	0
5	IOD	A	301	1/1	0.98	0.11	79,79,79,79	0
5	IOD	A	302	1/1	0.98	0.13	82,82,82,82	0
5	IOD	E	301	1/1	0.99	0.10	79,79,79,79	0
5	IOD	C	101	1/1	0.99	0.09	98,98,98,98	0
5	IOD	E	303	1/1	0.99	0.14	109,109,109,109	0
5	IOD	G	1000	1/1	0.99	0.07	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.