



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2016 – 05:21 AM EDT

PDB ID : 5DMK  
Title : Crystal Structure of IAg7 in complex with RLGL-WE14  
Authors : Wang, Y.; Jin, N.; Dai, S.; Kappler, J.W.  
Deposited on : 2015-09-08  
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

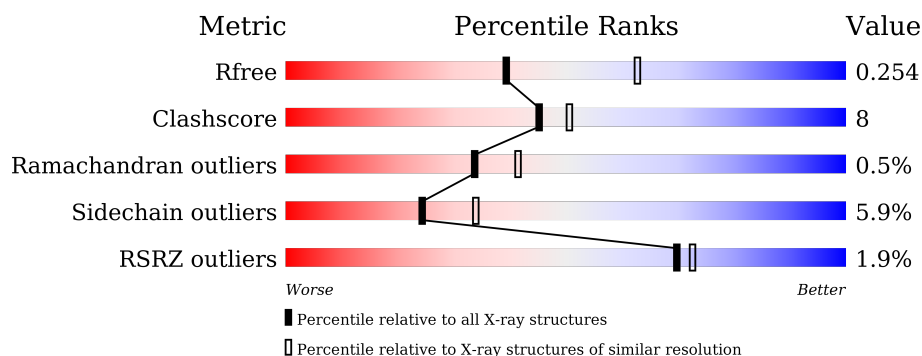
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	173	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	C	173	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>
1	E	173	<div> <div>3%</div> <div>79%</div> <div>21%</div> <div></div> </div>
1	G	173	<div> <div>4%</div> <div>79%</div> <div>20%</div> <div>•</div> </div>
2	B	212	<div> <div></div> <div>66%</div> <div>22%</div> <div>• 10%</div> </div>
2	D	212	<div> <div>%</div> <div>65%</div> <div>22%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	212	 71% 17% • 10%
2	H	212	 64% 24% • 11%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12200 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 H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1375	890	223	260	2			
1	C	173	Total	C	N	O	S	0	0	0
			1392	899	225	266	2			
1	E	173	Total	C	N	O	S	0	0	0
			1392	899	225	266	2			
1	G	173	Total	C	N	O	S	0	0	0
			1392	899	225	266	2			

- Molecule 2 is a protein called beta chain of Major Histocompatibility Complex Class II, I-Ag7,H2-Ab1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1585	996	286	296	7			
2	D	186	Total	C	N	O	S	0	0	0
			1550	977	276	290	7			
2	F	190	Total	C	N	O	S	0	0	0
			1580	993	284	296	7			
2	H	189	Total	C	N	O	S	0	0	0
			1575	990	283	295	7			

There are 32 discrepancies between the modelled and reference sequences:

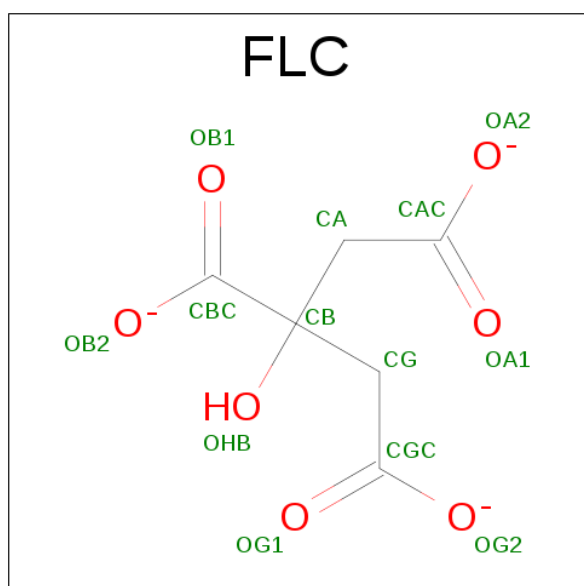
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	LEU	-	linker	PDB ?
B	-2	VAL	-	linker	PDB ?
B	-1	PRO	-	linker	PDB ?
B	0	ARG	-	linker	PDB ?
B	1	GLY	-	linker	PDB ?
B	2	SER	-	linker	PDB ?
B	3	GLY	-	linker	PDB ?
B	4	SER	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	LEU	-	linker	PDB ?
D	-2	VAL	-	linker	PDB ?
D	-1	PRO	-	linker	PDB ?
D	0	ARG	-	linker	PDB ?
D	1	GLY	-	linker	PDB ?
D	2	SER	-	linker	PDB ?
D	3	GLY	-	linker	PDB ?
D	4	SER	-	linker	PDB ?
F	-3	LEU	-	linker	PDB ?
F	-2	VAL	-	linker	PDB ?
F	-1	PRO	-	linker	PDB ?
F	0	ARG	-	linker	PDB ?
F	1	GLY	-	linker	PDB ?
F	2	SER	-	linker	PDB ?
F	3	GLY	-	linker	PDB ?
F	4	SER	-	linker	PDB ?
H	-3	LEU	-	linker	PDB ?
H	-2	VAL	-	linker	PDB ?
H	-1	PRO	-	linker	PDB ?
H	0	ARG	-	linker	PDB ?
H	1	GLY	-	linker	PDB ?
H	2	SER	-	linker	PDB ?
H	3	GLY	-	linker	PDB ?
H	4	SER	-	linker	PDB ?

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

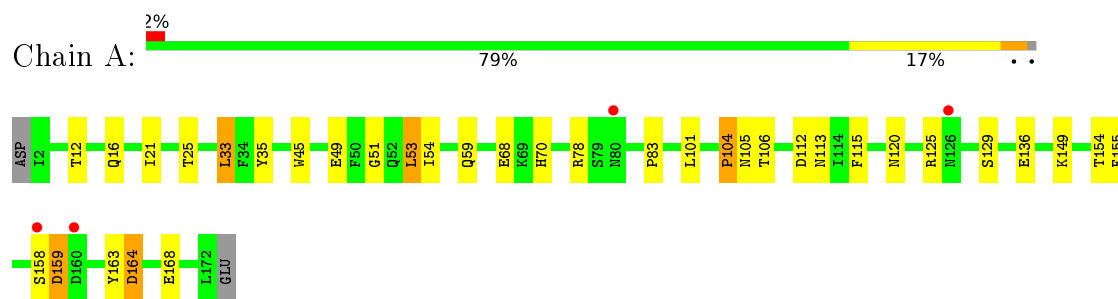
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	46	Total	O	0	0
			46	46		
4	C	29	Total	O	0	0
			29	29		
4	D	32	Total	O	0	0
			32	32		
4	E	46	Total	O	0	0
			46	46		
4	F	37	Total	O	0	0
			37	37		
4	G	52	Total	O	0	0
			52	52		
4	H	51	Total	O	0	0
			51	51		

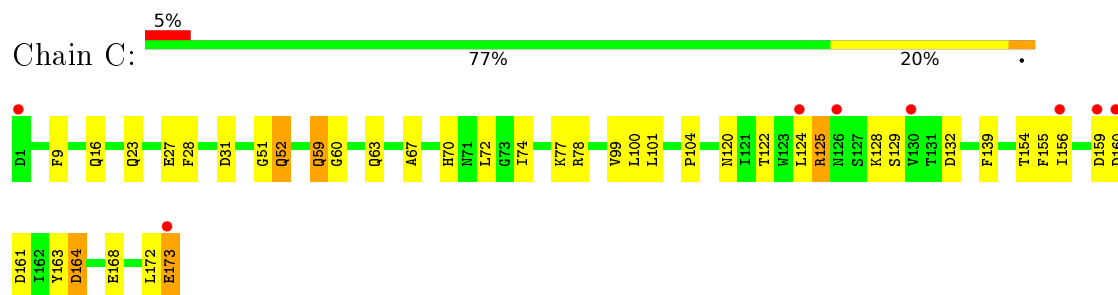
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

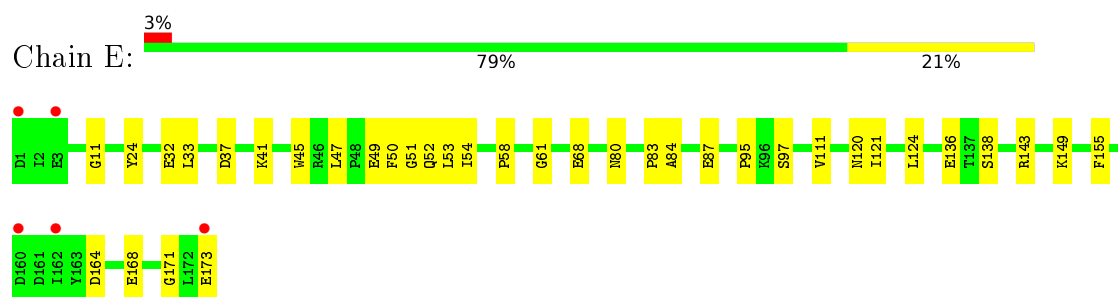
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain



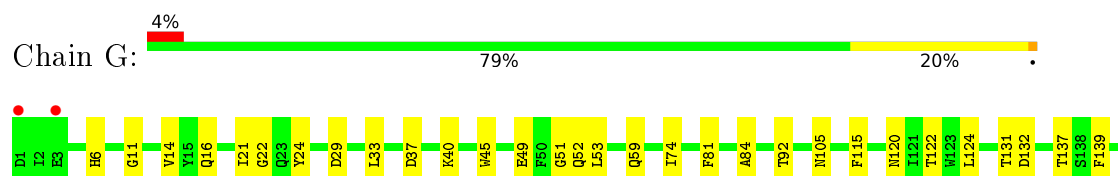
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain

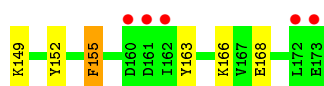


- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain



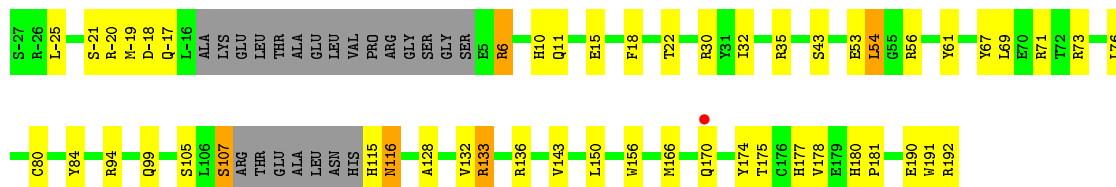
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain





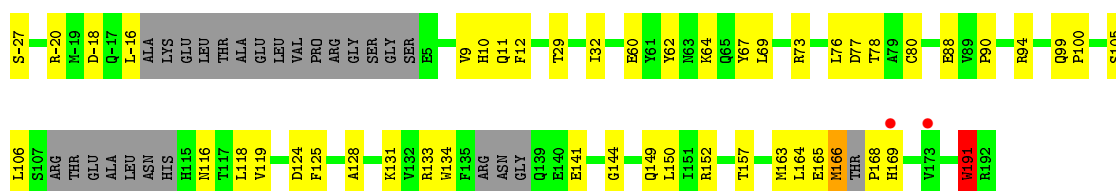
- Molecule 2: beta chain of Major Histocompatibility Complex Class II, I-Ag7,H2-Ab1 protein

Chain B: 66% 22% 10%



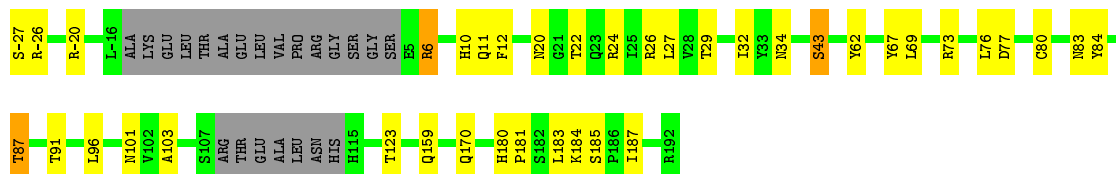
- Molecule 2: beta chain of Major Histocompatibility Complex Class II, I-Ag7,H2-Ab1 protein

Chain D: 65% 22% 12%



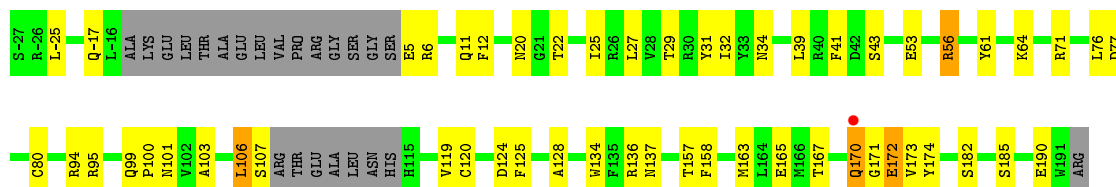
- Molecule 2: beta chain of Major Histocompatibility Complex Class II, I-Ag7,H2-Ab1 protein

Chain F: 71% 17% 10%



- Molecule 2: beta chain of Major Histocompatibility Complex Class II, I-Ag7,H2-Ab1 protein

Chain H: 64% 24% 11%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.76 Å   161.76 Å   204.16 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	44.87 – 2.45 45.73 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.6 (44.87-2.45) 93.6 (45.73-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.211   ,   0.260 0.204   ,   0.254	Depositor DCC
$R_{free}$ test set	4696 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 93210 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.46	0/1416	0.58	0/1932
1	C	0.44	0/1433	0.59	0/1955
1	E	0.45	0/1433	0.59	0/1955
1	G	0.46	0/1433	0.59	0/1955
2	B	0.47	0/1622	0.60	0/2196
2	D	0.49	1/1584 (0.1%)	0.62	1/2141 (0.0%)
2	F	0.46	0/1616	0.61	0/2188
2	H	0.45	0/1611	0.61	0/2181
All	All	0.46	1/12148 (0.0%)	0.60	1/16503 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	191	TRP	C-N	6.74	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	191	TRP	C-N-CA	-6.15	106.32	121.70

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	1375	0	1319	22	0
1	C	1392	0	1332	21	0
1	E	1392	0	1332	20	0
1	G	1392	0	1332	24	0
2	B	1585	0	1517	29	0
2	D	1550	0	1482	33	0
2	F	1580	0	1512	32	0
2	H	1575	0	1510	29	0
3	B	13	0	5	3	0
3	F	13	0	5	0	0
4	A	40	0	0	1	0
4	B	46	0	0	3	0
4	C	29	0	0	0	0
4	D	32	0	0	2	0
4	E	46	0	0	1	0
4	F	37	0	0	3	0
4	G	52	0	0	1	0
4	H	51	0	0	2	0
All	All	12200	0	11346	181	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 8.

All (181) 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:A:104:PRO:HB3	1:C:104:PRO:HB3	1.51	0.92
2:B:53:GLU:OE2	2:B:56:ARG:NH2	2.19	0.76
2:H:53:GLU:OE1	2:H:56:ARG:NH1	2.20	0.75
2:F:27:LEU:H	2:F:43:SER:HB3	1.54	0.72
1:A:53:LEU:HD13	1:A:54:ILE:HG13	1.72	0.71
2:F:11:GLN:HB2	2:F:32:ILE:HB	1.75	0.69
3:B:301:FLC:OA1	4:B:401:HOH:O	2.12	0.68
2:H:95:ARG:O	4:H:301:HOH:O	2.11	0.67
2:H:29:THR:HG21	4:H:303:HOH:O	1.95	0.66
2:B:136:ARG:HD3	2:B:174:TYR:HE1	1.61	0.66
2:F:83:ASN:O	2:F:87:THR:HG22	1.97	0.63
1:C:78:ARG:NH2	2:D:-18:ASP:OD2	2.30	0.62
1:E:68:GLU:OE1	2:F:10:HIS:ND1	2.25	0.62
1:E:45:TRP:HH2	2:F:-26:ARG:HD2	1.65	0.62
1:A:120:ASN:HB2	1:A:168:GLU:HB2	1.82	0.61
1:A:25:THR:HG22	1:A:35:TYR:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:SER:O	2:B:116:ASN:ND2	2.34	0.60
2:H:173:VAL:HG13	2:H:190:GLU:HG3	1.83	0.59
2:F:29:THR:HG21	4:F:407:HOH:O	2.03	0.58
2:D:131:LYS:HD3	2:D:133:ARG:CZ	2.34	0.58
1:G:81:PHE:O	2:H:6:ARG:NH2	2.36	0.58
1:E:80:ASN:ND2	4:E:204:HOH:O	2.36	0.57
2:H:12:PHE:HE1	2:H:29:THR:HG23	1.69	0.57
2:D:105:SER:OG	2:D:106:LEU:N	2.36	0.57
2:F:123:THR:HG22	2:F:159:GLN:HB2	1.85	0.57
2:B:11:GLN:HB2	2:B:32:ILE:HB	1.87	0.56
2:F:27:LEU:H	2:F:43:SER:CB	2.17	0.56
2:D:12:PHE:HE1	2:D:29:THR:HG23	1.71	0.56
1:A:83:PRO:HB3	2:B:6:ARG:HG2	1.88	0.56
2:F:76:LEU:O	2:F:80:CYS:HB2	2.06	0.55
1:E:52:GLN:HG2	2:H:103:ALA:HA	1.87	0.55
2:F:101:ASN:OD1	1:G:49:GLU:HG3	2.06	0.55
1:A:164:ASP:OD1	1:A:164:ASP:N	2.39	0.55
1:A:125:ARG:HD3	1:A:163:TYR:CE1	2.42	0.55
2:B:-20:ARG:NH1	3:B:301:FLC:OA2	2.32	0.54
2:F:87:THR:O	2:F:91:THR:OG1	2.24	0.54
2:F:184:LYS:HD3	2:H:94:ARG:HG2	1.90	0.54
1:E:37:ASP:O	1:E:41:LYS:N	2.40	0.54
2:H:11:GLN:HB2	2:H:32:ILE:HB	1.89	0.54
2:B:133:ARG:NH1	4:B:403:HOH:O	2.41	0.54
2:D:134:TRP:HB3	2:D:164:LEU:HD22	1.90	0.54
2:H:22:THR:HB	2:H:25:ILE:HD11	1.90	0.54
2:D:29:THR:HG21	4:D:307:HOH:O	2.08	0.53
2:H:119:VAL:HG22	2:H:163:MET:HG3	1.90	0.53
1:E:124:LEU:HB2	1:E:164:ASP:HB2	1.89	0.53
1:C:16:GLN:HG3	2:D:9:VAL:HG22	1.89	0.53
2:D:90:PRO:HA	2:D:94:ARG:HD3	1.91	0.53
2:F:184:LYS:NZ	4:F:403:HOH:O	2.35	0.53
1:G:6:HIS:ND1	1:G:29:ASP:OD2	2.42	0.53
1:G:16:GLN:HB3	1:G:21:ILE:HB	1.91	0.52
2:B:191:TRP:O	2:B:192:ARG:C	2.48	0.51
2:F:184:LYS:HG3	2:F:185:SER:N	2.26	0.51
2:D:76:LEU:O	2:D:80:CYS:HB2	2.11	0.51
2:F:69:LEU:HD11	2:F:73:ARG:HE	1.75	0.51
1:A:16:GLN:HG2	1:A:21:ILE:HD12	1.93	0.51
1:G:51:GLY:N	4:G:201:HOH:O	2.26	0.51
1:G:131:THR:HB	1:G:132:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:ND2	4:A:201:HOH:O	2.29	0.50
2:B:99:GLN:CD	2:D:99:GLN:HB2	2.32	0.50
2:H:12:PHE:CE1	2:H:29:THR:HG23	2.45	0.50
2:D:163:MET:N	2:D:163:MET:SD	2.85	0.50
2:B:143:VAL:HB	1:G:92:THR:HG21	1.94	0.50
2:D:11:GLN:HB2	2:D:32:ILE:HB	1.94	0.50
2:D:12:PHE:CE1	2:D:29:THR:HG23	2.47	0.50
1:G:37:ASP:OD2	1:G:40:LYS:HE3	2.12	0.50
1:E:83:PRO:HB3	2:F:6:ARG:HG2	1.93	0.49
2:F:12:PHE:HE1	2:F:29:THR:HG23	1.77	0.49
2:B:177:HIS:HD2	4:B:403:HOH:O	1.94	0.49
2:D:106:LEU:HD22	2:D:191:TRP:CH2	2.47	0.49
2:F:103:ALA:HA	1:G:52:GLN:HG2	1.94	0.49
1:A:105:ASN:HB3	1:A:155:PHE:CE1	2.47	0.49
1:A:45:TRP:CE2	1:A:51:GLY:HA3	2.48	0.49
1:C:9:PHE:HB2	1:C:27:GLU:HB2	1.94	0.48
2:B:99:GLN:NE2	2:D:99:GLN:HB2	2.29	0.48
2:D:-20:ARG:HB2	2:D:62:TYR:CE2	2.49	0.48
1:E:111:VAL:HG21	1:E:121:ILE:HD13	1.95	0.48
1:A:33:LEU:HD13	2:B:156:TRP:CZ2	2.49	0.47
1:G:139:PHE:CE1	1:G:149:LYS:HE3	2.49	0.47
2:H:99:GLN:HA	2:H:182:SER:OG	2.14	0.47
1:A:68:GLU:OE1	2:B:10:HIS:ND1	2.36	0.47
1:C:74:ILE:HG12	2:D:-16:LEU:HD23	1.96	0.47
1:E:120:ASN:HB2	1:E:168:GLU:HB2	1.96	0.47
2:B:-18:ASP:OD1	2:B:-17:GLN:N	2.41	0.47
1:E:47:LEU:HB2	1:E:50:PHE:CD2	2.50	0.47
2:B:-20:ARG:HD2	2:B:67:TYR:CD1	2.49	0.47
1:A:101:LEU:HD21	1:A:159:ASP:OD2	2.16	0.46
2:D:119:VAL:HG22	2:D:163:MET:HG3	1.96	0.46
1:E:11:GLY:HA2	1:E:24:TYR:CE1	2.50	0.46
1:A:125:ARG:HD3	1:A:163:TYR:CZ	2.51	0.46
2:F:187:ILE:HG23	1:G:53:LEU:HD21	1.97	0.46
2:B:191:TRP:HA	1:C:52:GLN:HB3	1.97	0.46
1:G:11:GLY:HA2	1:G:24:TYR:CZ	2.50	0.46
1:E:54:ILE:HG21	2:F:87:THR:OG1	2.15	0.46
2:H:31:TYR:HB2	2:H:39:LEU:HB3	1.97	0.46
2:D:116:ASN:ND2	2:D:168:PRO:HG3	2.31	0.46
2:F:-20:ARG:HB2	2:F:62:TYR:CE2	2.50	0.46
1:G:74:ILE:HD13	2:H:-17:GLN:O	2.16	0.46
2:F:27:LEU:HD13	2:F:80:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:180:HIS:CG	2:F:181:PRO:HD2	2.52	0.45
1:A:78:ARG:HD2	2:B:54:LEU:HD22	1.97	0.45
1:A:70:HIS:CD2	2:B:-19:MET:HG2	2.51	0.45
2:H:170:GLN:OE1	2:H:171:GLY:N	2.50	0.45
1:C:67:ALA:O	1:C:70:HIS:HB3	2.17	0.45
1:C:99:VAL:O	1:C:100:LEU:HD23	2.17	0.45
1:A:136:GLU:HG2	1:A:149:LYS:NZ	2.32	0.45
2:D:116:ASN:HD22	2:D:168:PRO:HG3	1.81	0.45
1:C:159:ASP:O	1:C:161:ASP:N	2.50	0.44
1:C:164:ASP:N	1:C:164:ASP:OD1	2.51	0.44
2:B:15:GLU:OE2	2:B:30:ARG:HD2	2.17	0.44
2:B:132:VAL:HG22	2:B:178:VAL:HG22	2.00	0.44
1:G:120:ASN:HB2	1:G:168:GLU:HB2	1.98	0.44
1:A:25:THR:HG22	1:A:35:TYR:CB	2.46	0.44
2:D:128:ALA:HB1	2:D:150:LEU:HD21	1.99	0.44
2:F:184:LYS:HG3	2:F:185:SER:H	1.82	0.44
2:H:136:ARG:HD3	2:H:174:TYR:CE1	2.53	0.44
2:B:18:PHE:CE2	2:B:84:TYR:HB2	2.53	0.44
2:H:128:ALA:HB2	2:H:158:PHE:CZ	2.52	0.44
1:C:128:LYS:HG2	1:C:129:SER:H	1.83	0.44
1:C:31:ASP:OD1	2:D:152:ARG:HD3	2.18	0.44
1:C:59:GLN:HG2	1:C:59:GLN:H	1.38	0.44
2:H:137:ASN:HD21	2:H:172:GLU:HA	1.83	0.44
2:B:76:LEU:O	2:B:80:CYS:HB2	2.17	0.44
1:C:120:ASN:HB2	1:C:168:GLU:HB2	1.99	0.44
2:F:180:HIS:CD2	2:F:181:PRO:HD2	2.53	0.43
1:G:14:VAL:O	1:G:22:GLY:HA2	2.17	0.43
1:A:115:PHE:CG	2:B:35:ARG:HD3	2.53	0.43
1:C:23:GLN:HE22	1:C:139:PHE:HB2	1.83	0.43
2:D:131:LYS:HD3	2:D:133:ARG:NH1	2.33	0.43
2:B:69:LEU:HD21	2:B:73:ARG:NH2	2.33	0.43
2:H:124:ASP:HA	2:H:157:THR:HB	2.01	0.43
2:F:12:PHE:CE1	2:F:29:THR:HG23	2.54	0.43
2:F:96:LEU:HD23	2:F:96:LEU:HA	1.81	0.43
1:G:137:THR:HG23	1:G:152:TYR:HE1	1.83	0.43
2:D:106:LEU:HD13	2:D:118:LEU:HD23	2.01	0.43
2:F:183:LEU:HB2	4:F:418:HOH:O	2.18	0.43
1:G:105:ASN:HB3	1:G:155:PHE:CE1	2.54	0.43
1:E:87:GLU:O	1:E:171:GLY:HA3	2.19	0.43
1:C:72:LEU:HD13	2:D:10:HIS:HB2	2.01	0.42
1:G:84:ALA:HB1	1:G:115:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:LEU:HG	2:H:107:SER:N	2.33	0.42
2:H:61:TYR:HA	2:H:64:LYS:HE2	2.01	0.42
2:D:141:GLU:HG3	2:D:164:LEU:HD21	2.02	0.42
1:G:166:LYS:NZ	1:G:168:GLU:OE2	2.53	0.42
1:C:60:GLY:HA2	1:C:63:GLN:OE1	2.20	0.42
2:B:128:ALA:HB1	2:B:150:LEU:HD21	2.01	0.42
1:E:95:PRO:HB2	1:E:97:SER:O	2.20	0.42
1:G:11:GLY:HA2	1:G:24:TYR:CE1	2.55	0.42
1:A:68:GLU:OE2	2:B:-21:SER:OG	2.37	0.42
2:D:-20:ARG:HB3	2:D:67:TYR:CE2	2.55	0.42
1:E:58:PRO:O	1:E:61:GLY:N	2.39	0.42
1:G:124:LEU:O	1:G:163:TYR:HA	2.20	0.42
1:G:45:TRP:CD1	1:G:51:GLY:HA3	2.55	0.42
1:C:125:ARG:HD2	1:C:163:TYR:OH	2.20	0.41
1:C:28:PHE:CE1	2:D:88:GLU:HG3	2.55	0.41
2:H:137:ASN:ND2	2:H:172:GLU:HA	2.35	0.41
1:A:112:ASP:OD1	1:A:113:ASN:N	2.45	0.41
1:E:136:GLU:OE1	1:E:149:LYS:NZ	2.36	0.41
1:E:49:GLU:HG3	2:H:101:ASN:OD1	2.21	0.41
2:F:22:THR:HG23	2:F:84:TYR:CD1	2.55	0.41
1:C:172:LEU:HB3	1:C:173:GLU:H	1.55	0.41
2:D:100:PRO:HB3	2:D:125:PHE:HB3	2.01	0.41
2:D:144:GLY:N	4:D:301:HOH:O	2.21	0.41
2:F:180:HIS:HA	2:F:181:PRO:HD3	1.94	0.41
2:F:-20:ARG:HB3	2:F:67:TYR:CE2	2.55	0.41
2:H:100:PRO:HB3	2:H:125:PHE:HB3	2.02	0.41
2:H:29:THR:HB	2:H:41:PHE:HB3	2.02	0.41
2:B:180:HIS:CG	2:B:181:PRO:HD2	2.56	0.41
1:G:45:TRP:NE1	1:G:51:GLY:HA3	2.35	0.41
2:H:76:LEU:O	2:H:80:CYS:HB2	2.21	0.41
3:B:301:FLC:OHB	3:B:301:FLC:OA1	2.35	0.41
1:G:139:PHE:CZ	1:G:149:LYS:HE3	2.56	0.41
2:D:69:LEU:HD21	2:D:73:ARG:NH2	2.36	0.41
1:E:32:GLU:OE2	1:E:138:SER:OG	2.22	0.40
2:H:27:LEU:HB3	2:H:43:SER:HB3	2.02	0.40
2:H:120:CYS:HB2	2:H:134:TRP:CZ2	2.57	0.40
1:C:125:ARG:HH11	1:C:125:ARG:HB3	1.86	0.40
2:D:116:ASN:OD1	2:D:166:MET:HG3	2.20	0.40
2:D:124:ASP:HA	2:D:157:THR:HB	2.02	0.40
1:E:45:TRP:CD1	1:E:51:GLY:HA3	2.56	0.40
1:E:84:ALA:HB2	2:F:34:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:-17:GLN:HB3	2:B:61:TYR:CZ	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	169/173 (98%)	159 (94%)	9 (5%)	1 (1%)	30	35
1	C	171/173 (99%)	161 (94%)	7 (4%)	3 (2%)	11	9
1	E	171/173 (99%)	161 (94%)	10 (6%)	0	100	100
1	G	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
2	B	184/212 (87%)	171 (93%)	13 (7%)	0	100	100
2	D	176/212 (83%)	168 (96%)	7 (4%)	1 (1%)	30	35
2	F	184/212 (87%)	176 (96%)	8 (4%)	0	100	100
2	H	183/212 (86%)	174 (95%)	7 (4%)	2 (1%)	17	19
All	All	1409/1540 (92%)	1338 (95%)	64 (4%)	7 (0%)	34	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	GLN
1	C	160	ASP
2	D	169	HIS
2	H	34	ASN
2	H	172	GLU
1	A	104	PRO
1	C	51	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	153/155 (99%)	142 (93%)	11 (7%)	18	24
1	C	155/155 (100%)	143 (92%)	12 (8%)	16	21
1	E	155/155 (100%)	150 (97%)	5 (3%)	46	63
1	G	155/155 (100%)	151 (97%)	4 (3%)	54	70
2	B	174/192 (91%)	158 (91%)	16 (9%)	11	13
2	D	170/192 (88%)	161 (95%)	9 (5%)	28	39
2	F	173/192 (90%)	164 (95%)	9 (5%)	29	40
2	H	173/192 (90%)	162 (94%)	11 (6%)	22	29
All	All	1308/1388 (94%)	1231 (94%)	77 (6%)	24	34

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	33	LEU
1	A	49	GLU
1	A	53	LEU
1	A	59	GLN
1	A	106	THR
1	A	129	SER
1	A	154	THR
1	A	158	SER
1	A	159	ASP
1	A	164	ASP
2	B	-25	LEU
2	B	6	ARG
2	B	22	THR
2	B	43	SER
2	B	54	LEU
2	B	71	ARG
2	B	94	ARG
2	B	105	SER

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Mol	Chain	Res	Type
2	B	107	SER
2	B	115	HIS
2	B	116	ASN
2	B	133	ARG
2	B	166	MET
2	B	170	GLN
2	B	175	THR
2	B	190	GLU
1	C	59	GLN
1	C	77	LYS
1	C	101	LEU
1	C	122	THR
1	C	124	LEU
1	C	125	ARG
1	C	132	ASP
1	C	154	THR
1	C	155	PHE
1	C	156	ILE
1	C	164	ASP
1	C	173	GLU
2	D	-27	SER
2	D	60	GLU
2	D	64	LYS
2	D	77	ASP
2	D	78	THR
2	D	149	GLN
2	D	165	GLU
2	D	166	MET
2	D	191	TRP
1	E	33	LEU
1	E	53	LEU
1	E	143	ARG
1	E	155	PHE
1	E	173	GLU
2	F	-27	SER
2	F	6	ARG
2	F	20	ASN
2	F	24	ARG
2	F	26	ARG
2	F	43	SER
2	F	77	ASP
2	F	87	THR

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Mol	Chain	Res	Type
2	F	170	GLN
1	G	33	LEU
1	G	59	GLN
1	G	122	THR
1	G	155	PHE
2	H	-25	LEU
2	H	5	GLU
2	H	20	ASN
2	H	56	ARG
2	H	71	ARG
2	H	77	ASP
2	H	106	LEU
2	H	165	GLU
2	H	167	THR
2	H	170	GLN
2	H	185	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	116	ASN

### 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	$\# Z  > 2$
3	FLC	B	301	-	3,12,12	1.11	0	3,17,17	2.53	1 (33%)
3	FLC	F	301	-	3,12,12	0.63	0	3,17,17	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	B	301	-	-	0/6/16/16	0/0/0/0
3	FLC	F	301	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	FLC	CB-CA-CAC	-4.33	108.18	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	FLC	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	171/173 (98%)	-0.07	4 (2%) 64 66	31, 44, 75, 96	0
1	C	173/173 (100%)	0.03	8 (4%) 36 40	33, 47, 85, 109	0
1	E	173/173 (100%)	-0.06	5 (2%) 55 58	33, 44, 70, 93	0
1	G	173/173 (100%)	-0.06	7 (4%) 42 45	32, 43, 72, 90	0
2	B	190/212 (89%)	-0.29	1 (0%) 91 92	31, 43, 69, 96	0
2	D	186/212 (87%)	-0.15	2 (1%) 82 84	33, 48, 78, 110	0
2	F	190/212 (89%)	-0.29	0 100 100	32, 45, 68, 86	0
2	H	189/212 (89%)	-0.29	1 (0%) 91 92	32, 44, 67, 111	0
All	All	1445/1540 (93%)	-0.15	28 (1%) 70 72	31, 45, 75, 111	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	ASP	5.2
1	C	130	VAL	4.7
1	E	160	ASP	4.3
1	G	1	ASP	4.2
2	H	170	GLN	4.1
1	G	3	GLU	4.0
1	G	160	ASP	3.9
1	C	173	GLU	3.8
1	A	160	ASP	3.5
1	E	3	GLU	3.2
1	C	159	ASP	3.0
1	G	162	ILE	2.8
1	G	173	GLU	2.6
1	E	162	ILE	2.5
1	E	173	GLU	2.5
2	D	173	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	124	LEU	2.3
2	B	170	GLN	2.3
1	A	158	SER	2.3
1	A	126	ASN	2.2
2	D	169	HIS	2.2
1	G	161	ASP	2.1
1	E	1	ASP	2.1
1	C	1	ASP	2.1
1	G	172	LEU	2.1
1	C	126	ASN	2.1
1	C	156	ILE	2.0
1	A	80	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FLC	F	301	13/13	0.95	0.14	-0.83	54,56,66,69	0
3	FLC	B	301	13/13	0.94	0.12	-0.98	41,51,58,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.