



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 08:02 AM BST

PDB ID : 6T3J  
Title : Dual Epitope Targeting by Anti-DR5 Antibodies  
Authors : Tauchert, M.J.; Augustin, M.; Krapp, S.; Overdijk, M.B.; Breij, E.C.W.; Hibbert, R.G.  
Deposited on : 2019-10-11  
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

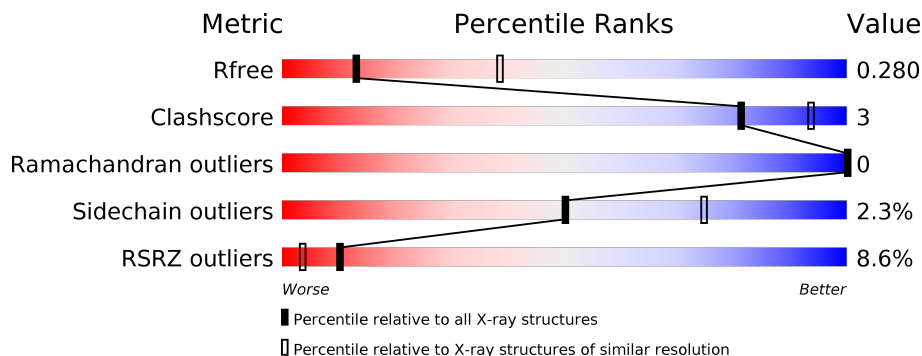
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

# 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 3.05 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.



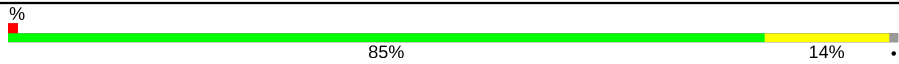

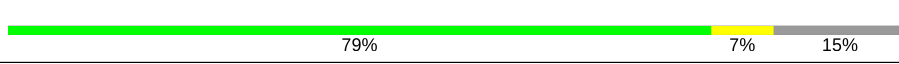
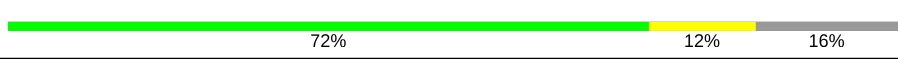
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	232	
1	F	232	
2	B	214	
2	G	214	
3	C	232	
3	H	232	

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Mol	Chain	Length	Quality of chain
4	D	213	 <p>% 85% 14%</p>
4	I	213	 <p>29% 88% 10%</p>
5	E	131	 <p>79% 7% 15%</p>
5	J	131	 <p>72% 12% 16%</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14837 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 IgG1-hDR5-01-Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	Total	C	N	O	S	32	0	0
			1654	1048	273	328	5			
1	F	219	Total	C	N	O	S	43	0	0
			1654	1048	273	328	5			

- Molecule 2 is a protein called IgG1-hDR5-01-Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	Total	C	N	O	S	34	0	0
			1632	1022	278	327	5			
2	G	213	Total	C	N	O	S	39	0	0
			1641	1027	279	330	5			

- Molecule 3 is a protein called IgG1-hDR5-05-Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	219	Total	C	N	O	S	39	0	0
			1653	1040	284	323	6			
3	H	218	Total	C	N	O	S	6	0	0
			1644	1035	282	321	6			

- Molecule 4 is a protein called IgG1-hDR5-05-Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
4	D	210	Total	C	N	O	P	S	42	0	0
			1624	1018	269	331	1	5			
4	I	210	Total	C	N	O	P	S	13	0	0
			1624	1018	269	331	1	5			

- Molecule 5 is a protein called Tumor necrosis factor receptor superfamily member 10B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	112	863	514	157	176	16	13	0	0
5	J	110	848	506	152	174	16	25	0	0

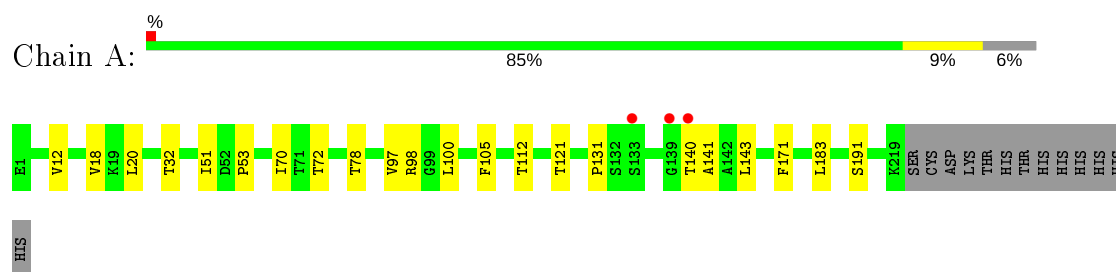
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	185	GLU	-	expression tag	UNP O14763
E	186	PRO	-	expression tag	UNP O14763
E	187	GLU	-	expression tag	UNP O14763
E	188	ALA	-	expression tag	UNP O14763
J	185	GLU	-	expression tag	UNP O14763
J	186	PRO	-	expression tag	UNP O14763
J	187	GLU	-	expression tag	UNP O14763
J	188	ALA	-	expression tag	UNP O14763

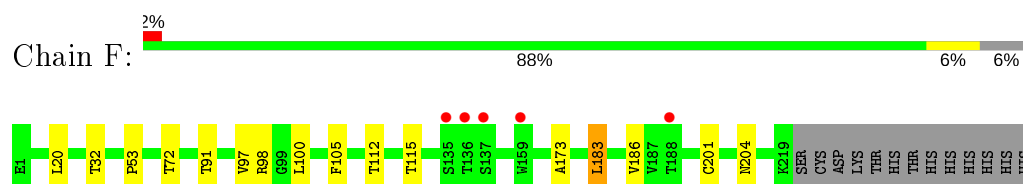
### 3 Residue-property plots

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.

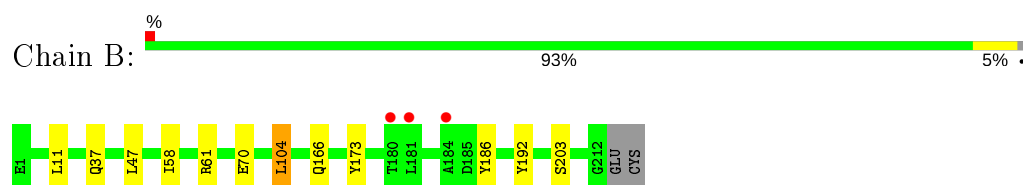
- Molecule 1: IgG1-hDR5-01-Heavy Chain



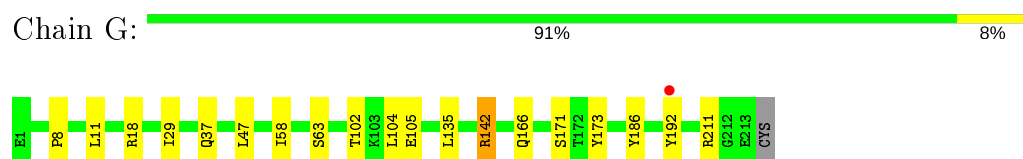
- Molecule 1: IgG1-hDR5-01-Heavy Chain



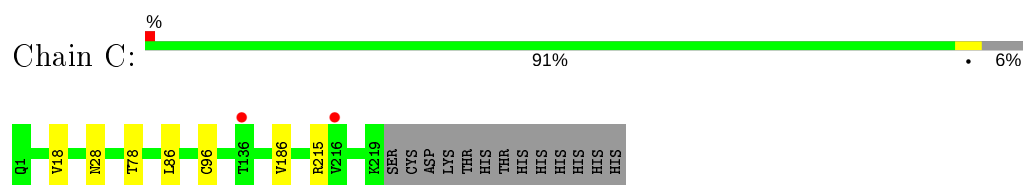
- Molecule 2: IgG1-hDR5-01-Light Chain



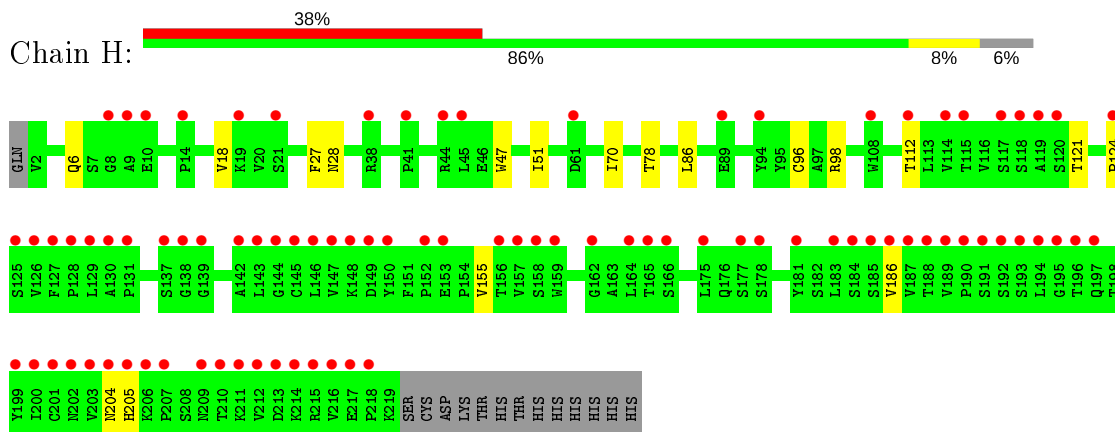
- Molecule 2: IgG1-hDR5-01-Light Chain



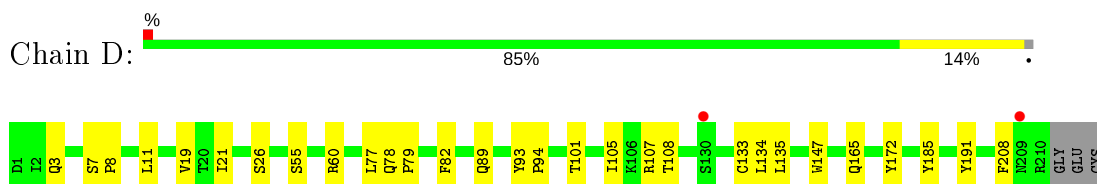
- Molecule 3: IgG1-hDR5-05-Heavy Chain



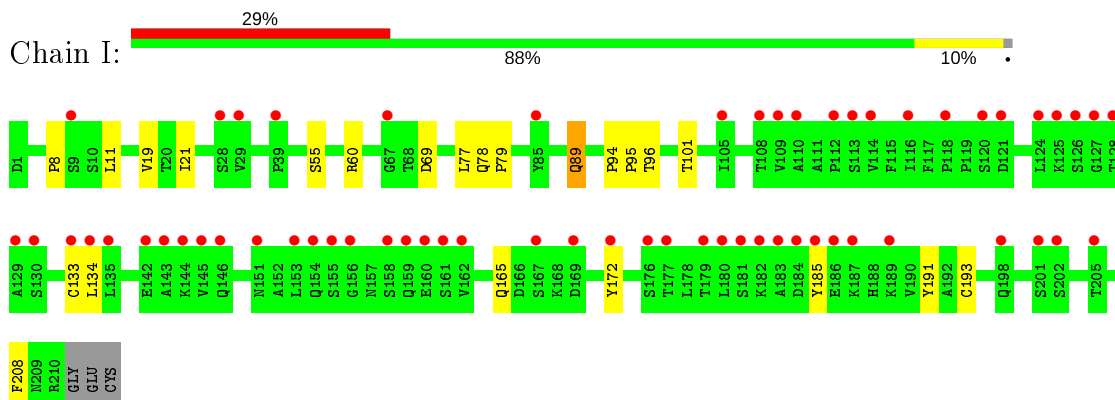
- Molecule 3: IgG1-hDR5-05-Heavy Chain



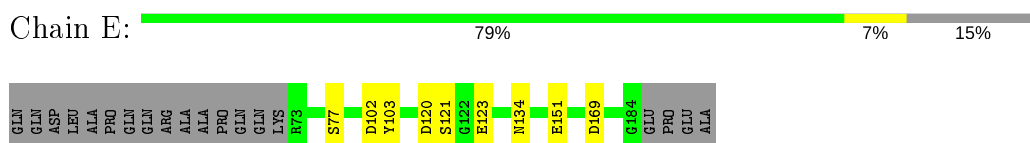
- Molecule 4: IgG1-hDR5-05-Light Chain



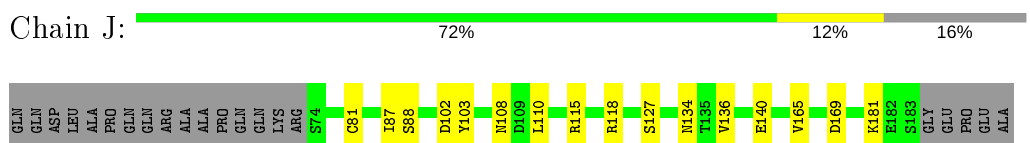
- Molecule 4: IgG1-hDR5-05-Light Chain



- Molecule 5: Tumor necrosis factor receptor superfamily member 10B



- Molecule 5: Tumor necrosis factor receptor superfamily member 10B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.60Å 90.93Å 138.38Å 90.00° 103.79° 90.00°	Depositor
Resolution (Å)	134.41 – 3.05 45.92 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (134.41-3.05) 98.5 (45.92-3.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.06Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.251 , 0.282 0.252 , 0.280	Depositor DCC
$R_{free}$ test set	534 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.1	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: SEP

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	0.48	0/1695	0.72	1/2312 (0.0%)
1	F	0.46	0/1695	0.71	1/2312 (0.0%)
2	B	0.51	1/1668 (0.1%)	0.71	0/2264
2	G	0.66	3/1677 (0.2%)	0.70	1/2276 (0.0%)
3	C	0.46	0/1693	0.72	1/2308 (0.0%)
3	H	0.43	0/1684	0.69	0/2296
4	D	0.48	0/1654	0.67	0/2249
4	I	0.44	0/1654	0.67	0/2249
5	E	0.47	0/881	0.75	0/1189
5	J	0.60	1/866 (0.1%)	0.95	6/1170 (0.5%)
All	All	0.50	5/15167 (0.0%)	0.72	10/20625 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	211	ARG	NE-CZ	14.79	1.52	1.33
2	G	142	ARG	NE-CZ	11.24	1.47	1.33
5	J	140	GLU	CG-CD	-10.25	1.36	1.51
2	B	70	GLU	CG-CD	7.46	1.63	1.51
2	G	18	ARG	NE-CZ	6.52	1.41	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	118	ARG	NE-CZ-NH2	9.60	125.10	120.30
5	J	118	ARG	NE-CZ-NH1	-9.13	115.74	120.30
5	J	118	ARG	CD-NE-CZ	8.85	135.99	123.60
1	A	140	THR	CA-CB-CG2	6.58	121.61	112.40
2	G	211	ARG	NE-CZ-NH1	6.03	123.31	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	142	ARG	Sidechain

## 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	1654	0	1625	11	0
1	F	1654	0	1625	9	0
2	B	1632	0	1590	4	0
2	G	1641	0	1596	6	0
3	C	1653	0	1624	3	0
3	H	1644	0	1613	12	0
4	D	1624	0	1560	14	0
4	I	1624	0	1562	13	0
5	E	863	0	782	2	0
5	J	848	0	766	7	0
All	All	14837	0	14343	74	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.

The worst 5 of 74 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:97:VAL:CG1	1:A:105:PHE:HB3	2.32	0.60
3:H:47:TRP:CZ3	4:I:94:PRO:HB3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:THR:HG23	1:F:115:THR:HA	1.87	0.56
4:D:107:ARG:HG2	4:D:108:THR:N	2.19	0.56
3:C:186:VAL:HG11	4:D:134:LEU:CD2	2.36	0.56

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	217/232 (94%)	210 (97%)	7 (3%)	0	100	100
1	F	217/232 (94%)	212 (98%)	5 (2%)	0	100	100
2	B	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
2	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
3	C	217/232 (94%)	212 (98%)	5 (2%)	0	100	100
3	H	216/232 (93%)	208 (96%)	8 (4%)	0	100	100
4	D	207/213 (97%)	198 (96%)	9 (4%)	0	100	100
4	I	207/213 (97%)	198 (96%)	9 (4%)	0	100	100
5	E	110/131 (84%)	97 (88%)	13 (12%)	0	100	100
5	J	108/131 (82%)	96 (89%)	12 (11%)	0	100	100
All	All	1920/2044 (94%)	1835 (96%)	85 (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	187/200 (94%)	184 (98%)	3 (2%)	62	83
1	F	187/200 (94%)	184 (98%)	3 (2%)	62	83
2	B	185/187 (99%)	181 (98%)	4 (2%)	52	76
2	G	186/187 (100%)	181 (97%)	5 (3%)	44	71
3	C	185/198 (93%)	182 (98%)	3 (2%)	62	83
3	H	184/198 (93%)	179 (97%)	5 (3%)	44	71
4	D	185/187 (99%)	181 (98%)	4 (2%)	52	76
4	I	185/187 (99%)	181 (98%)	4 (2%)	52	76
5	E	102/117 (87%)	97 (95%)	5 (5%)	25	55
5	J	101/117 (86%)	99 (98%)	2 (2%)	55	78
All	All	1687/1778 (95%)	1649 (98%)	38 (2%)	50	75

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	151	GLU
1	F	204	ASN
4	I	208	PHE
1	F	98	ARG
2	G	29	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	138	GLN
4	I	123	GLN
3	H	205	HIS
4	D	88	GLN
1	F	169	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](#)

2 non-standard protein/DNA/RNA residues 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
4	SEP	I	55	4	8,9,10	0.63	0	8,12,14	1.52	2 (25%)
4	SEP	D	55	4	8,9,10	0.81	0	8,12,14	1.80	1 (12%)

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
4	SEP	I	55	4	-	1/5/8/10	-
4	SEP	D	55	4	-	2/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	D	55	SEP	P-OG-CB	3.99	129.28	118.30
4	I	55	SEP	P-OG-CB	3.07	126.75	118.30
4	I	55	SEP	OG-P-O1P	-2.02	100.81	106.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	55	SEP	N-CA-CB-OG
4	D	55	SEP	N-CA-CB-OG
4	D	55	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	219/232 (94%)	-0.21	3 (1%) 75 53	51, 97, 156, 231	17 (7%)
1	F	219/232 (94%)	-0.10	5 (2%) 60 36	50, 109, 176, 226	20 (9%)
2	B	212/214 (99%)	-0.33	3 (1%) 75 53	47, 78, 151, 209	14 (6%)
2	G	213/214 (99%)	-0.36	1 (0%) 91 79	52, 92, 165, 194	17 (7%)
3	C	219/232 (94%)	-0.30	2 (0%) 84 66	61, 111, 167, 263	19 (8%)
3	H	218/232 (93%)	2.37	89 (40%) 0 0	140, 237, 535, 689	3 (1%)
4	D	209/213 (98%)	-0.23	2 (0%) 82 63	45, 104, 169, 188	20 (9%)
4	I	209/213 (98%)	1.62	61 (29%) 0 0	85, 217, 384, 608	5 (2%)
5	E	112/131 (85%)	-0.41	0 100 100	47, 70, 139, 198	5 (4%)
5	J	110/131 (83%)	-0.36	0 100 100	51, 76, 132, 161	9 (8%)
All	All	1940/2044 (94%)	0.23	166 (8%) 10 4	45, 109, 321, 689	129 (6%)

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	181	SER	17.3
3	H	203	VAL	14.9
3	H	125	SER	14.7
3	H	188	THR	13.4
3	H	186	VAL	12.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	SEP	I	55	10/11	0.86	0.24	106,114,124,134	0
4	SEP	D	55	10/11	0.96	0.20	53,65,75,79	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.