



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 PM UTC

PDB ID : 6T3J / pdb_00006t3j
Title : Dual Epitope Targeting by Anti-DR5 Antibodies
Authors : Tauchert, M.J.; Augustin, M.; Krapp, S.; Overdijk, M.B.; Breij, E.C.W.; Hilbert, R.G.
Deposited on : 2019-10-11
Resolution : 3.05 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

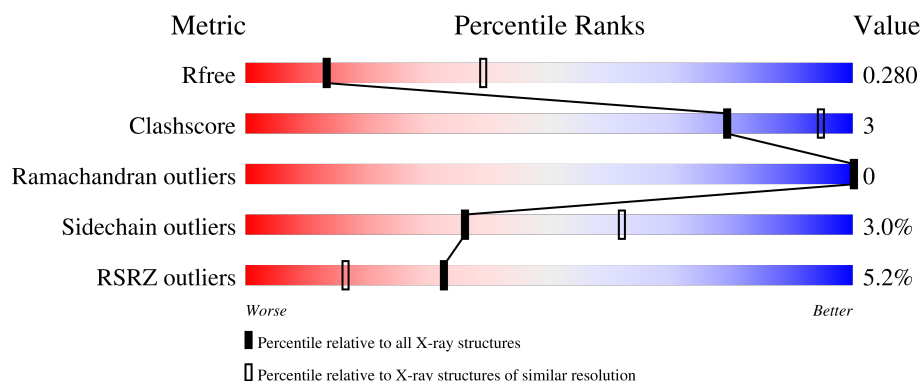
1 Overall quality at a glance

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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	5% 83% 11% 6%
1	F	232	4% 86% 9% 6%
2	B	214	% 93% 6% .
2	G	214	% 91% 8% .
3	C	232	2% 90% 6% .

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Mol	Chain	Length	Quality of chain
3	H	232	19% 85% 9% 6%
4	D	213	3% 86% 13%
4	I	213	8% 88% 10%
5	E	131	% 79% 7% 15%
5	J	131	% 73% 11% 16%

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
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
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
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
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
5	E	112	Total 863	C 514	N 157	O 176	S 16	13	0	0
5	J	110	Total 848	C 506	N 152	O 174	S 16	25	0	0

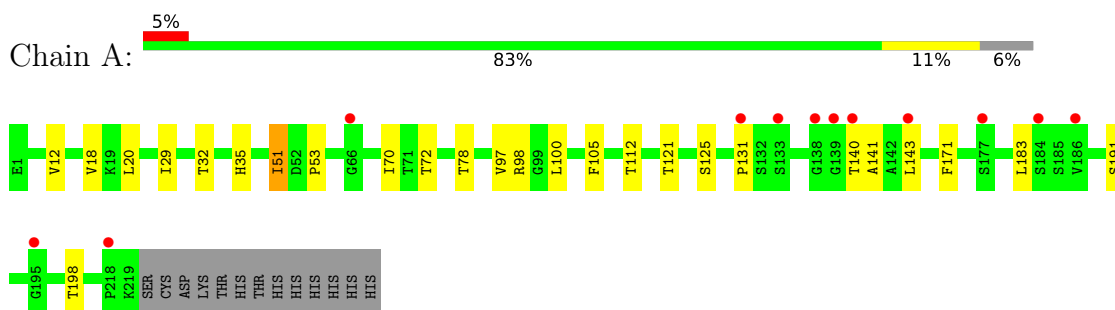
There are 8 discrepancies between the modelled and reference sequences:

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

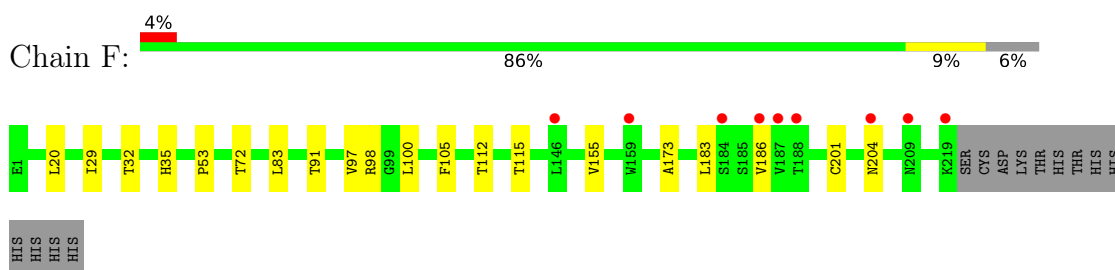
3 Residue-property plots [i](#)

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.

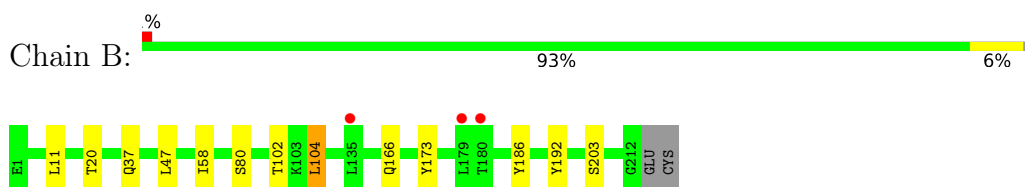
- Molecule 1: IgG1-hDR5-01-Heavy Chain



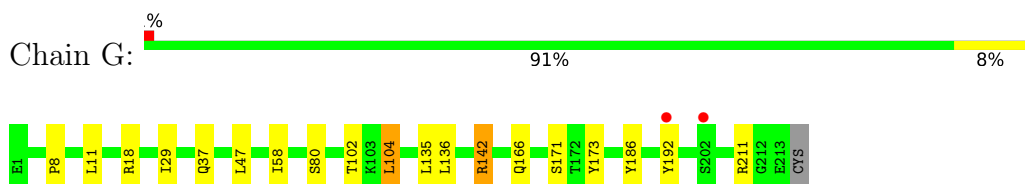
- Molecule 1: IgG1-hDR5-01-Heavy Chain



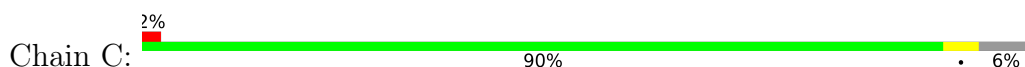
- Molecule 2: IgG1-hDR5-01-Light Chain



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

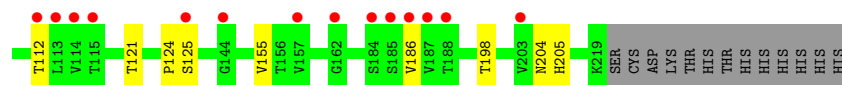
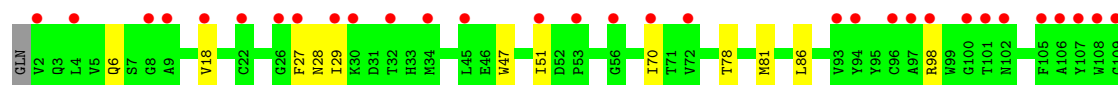
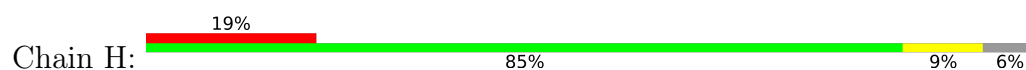


- Molecule 3: IgG1-hDR5-05-Heavy Chain

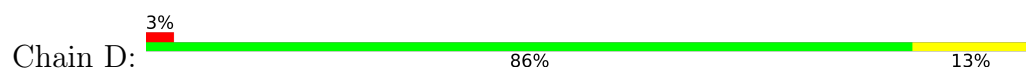




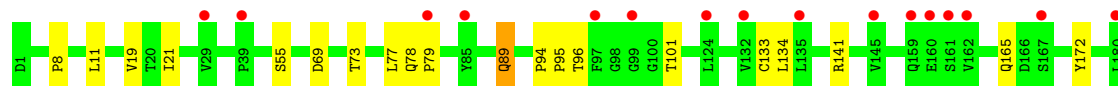
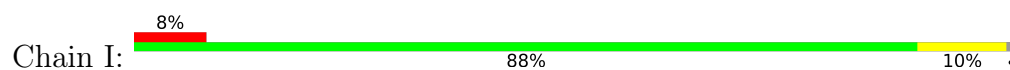
• Molecule 3: IgG1-hDR5-05-Heavy Chain



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



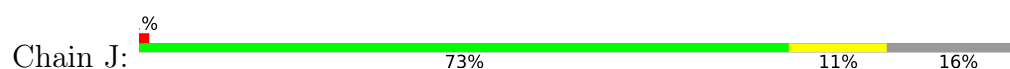
• Molecule 4: IgG1-hDR5-05-Light Chain



• 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, α , β , γ	121.60Å 90.93Å 138.38Å 90.00° 103.79° 90.00°	Depositor
Resolution (Å)	134.41 – 3.05 134.39 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (134.41-3.05) 98.5 (134.39-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.06Å)	Xtriage
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 (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	86.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 82.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14837	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.66	0/1695	0.88	2/2312 (0.1%)
1	F	0.64	0/1695	0.87	0/2312
2	B	0.64	0/1668	0.86	0/2264
2	G	0.84	3/1677 (0.2%)	0.84	0/2276
3	C	0.62	1/1693 (0.1%)	0.87	1/2308 (0.0%)
3	H	0.63	0/1684	0.85	0/2296
4	D	0.62	0/1654	0.82	0/2249
4	I	0.61	0/1654	0.83	1/2249 (0.0%)
5	E	0.61	0/881	0.88	0/1189
5	J	0.72	2/866 (0.2%)	1.04	5/1170 (0.4%)
All	All	0.66	6/15167 (0.0%)	0.87	9/20625 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	211	ARG	NE-CZ	17.48	1.52	1.33
2	G	142	ARG	NE-CZ	13.28	1.47	1.33
2	G	18	ARG	NE-CZ	7.71	1.41	1.33
5	J	140	GLU	CG-CD	-6.19	1.36	1.52
5	J	118	ARG	NE-CZ	-5.60	1.26	1.33
3	C	87	ARG	NE-CZ	5.44	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	140	GLU	CB-CG-CD	8.35	126.80	112.60
5	J	118	ARG	CD-NE-CZ	8.28	135.99	124.40
5	J	118	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	A	140	THR	CA-CB-CG2	6.53	121.61	110.50
5	J	118	ARG	NE-CZ-NH1	-5.76	115.74	121.50
4	I	141	ARG	CB-CA-C	-5.68	101.02	110.68
1	A	51	ILE	CB-CG1-CD1	-5.66	101.91	113.80
3	C	13	LYS	CG-CD-CE	5.41	123.74	111.30
5	J	171	THR	CB-CA-C	5.19	117.11	109.22

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

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	13	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	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (75) 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
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
1:A:12:VAL:HG21	1:A:18:VAL:HG22	1.87	0.55
1:A:12:VAL:HG21	1:A:18:VAL:CG2	2.36	0.55
1:F:97:VAL:CG1	1:F:105:PHE:HB3	2.37	0.55
4:D:134:LEU:HD12	4:D:135:LEU:N	2.24	0.53
5:J:103:TYR:CZ	5:J:134:ASN:HB2	2.43	0.53
4:I:94:PRO:O	4:I:96:THR:HG23	2.09	0.53
1:A:141:ALA:HB2	1:A:191:SER:HB3	1.91	0.53
1:F:173:ALA:HB2	1:F:183:LEU:HD23	1.91	0.52
5:J:81:CYS:SG	5:J:87:ILE:HG13	2.50	0.51
5:E:103:TYR:CZ	5:E:134:ASN:HB2	2.46	0.51
1:A:32:THR:HG22	1:A:100:LEU:HD23	1.92	0.51
2:G:11:LEU:HB3	2:G:104:LEU:HD22	1.92	0.51
5:J:87:ILE:HG22	5:J:88:SER:O	2.10	0.51
4:D:93:TYR:CD1	4:D:94:PRO:HA	2.46	0.50
3:H:6:GLN:HE21	3:H:112:THR:HG23	1.77	0.50
1:F:32:THR:HG22	1:F:100:LEU:HD23	1.93	0.49
1:A:97:VAL:HG11	1:A:105:PHE:CG	2.47	0.49
3:H:124:PRO:HG3	3:H:205:HIS:NE2	2.27	0.49
3:H:47:TRP:CD2	4:I:95:PRO:HD2	2.48	0.48
4:I:78:GLN:HB3	4:I:79:PRO:HD2	1.96	0.48
2:B:11:LEU:HB3	2:B:104:LEU:HD22	1.95	0.48
4:I:19:VAL:HG21	4:I:77:LEU:HD11	1.95	0.48
4:D:19:VAL:HG21	4:D:77:LEU:HD11	1.95	0.48
4:D:78:GLN:HB3	4:D:79:PRO:HD2	1.95	0.48
4:I:89:GLN:O	4:I:89:GLN:NE2	2.47	0.47
1:A:171:PHE:O	1:A:183:LEU:HD21	2.15	0.47
2:B:186:TYR:O	2:B:192:TYR:OH	2.34	0.46
2:G:186:TYR:O	2:G:192:TYR:OH	2.32	0.46
3:H:27:PHE:CE2	3:H:98:ARG:HD2	2.51	0.46
3:H:124:PRO:HG3	3:H:205:HIS:CD2	2.50	0.46
3:C:186:VAL:HG11	4:D:134:LEU:HD22	1.98	0.45
3:H:47:TRP:CE2	4:I:95:PRO:HD2	2.51	0.45
3:H:186:VAL:HG11	4:I:134:LEU:HD22	1.99	0.45
5:J:108:ASN:HB2	5:J:110:LEU:HD13	1.99	0.45
3:H:51:ILE:HD11	3:H:70:ILE:C	2.42	0.45
3:H:51:ILE:HD11	3:H:70:ILE:O	2.17	0.45
3:H:155:VAL:HG22	3:H:205:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:LEU:HD22	1:F:112:THR:HG21	1.99	0.44
4:D:21:ILE:CG2	4:D:101:THR:HG21	2.48	0.44
4:D:82:PHE:CZ	4:D:105:ILE:HG12	2.52	0.44
5:E:120:ASP:HB2	5:E:123:GLU:OE1	2.17	0.44
4:D:185:TYR:O	4:D:191:TYR:OH	2.36	0.44
5:J:127:SER:HB3	5:J:136:VAL:HB	1.99	0.44
4:I:133:CYS:HG	4:I:193:CYS:CB	2.24	0.44
1:A:20:LEU:HD22	1:A:112:THR:HG21	2.00	0.44
4:I:185:TYR:O	4:I:191:TYR:OH	2.36	0.44
1:A:53:PRO:HB3	1:A:72:THR:HG21	2.00	0.44
2:B:166:GLN:HG3	2:B:173:TYR:CZ	2.54	0.43
2:G:37:GLN:HB2	2:G:47:LEU:HD11	2.00	0.43
1:F:53:PRO:HB3	1:F:72:THR:HG21	2.00	0.43
1:F:97:VAL:HG11	1:F:105:PHE:CG	2.54	0.43
4:I:165:GLN:HG3	4:I:172:TYR:CZ	2.53	0.43
1:A:51:ILE:HG21	1:A:70:ILE:HB	2.01	0.43
5:J:165:VAL:HG23	5:J:181:LYS:HG2	2.01	0.43
4:I:8:PRO:HG2	4:I:11:LEU:HG	2.00	0.42
1:F:173:ALA:HA	1:F:183:LEU:HB3	2.01	0.42
4:I:21:ILE:HG23	4:I:101:THR:HG21	2.00	0.42
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.00	0.42
2:G:8:PRO:O	2:G:102:THR:HG23	2.20	0.42
3:H:155:VAL:HG13	3:H:205:HIS:CD2	2.55	0.42
5:J:87:ILE:CG2	5:J:88:SER:O	2.68	0.41
2:G:166:GLN:HG3	2:G:173:TYR:CZ	2.56	0.41
1:A:131:PRO:HD3	1:A:143:LEU:CD2	2.51	0.41
4:D:165:GLN:HG3	4:D:172:TYR:CZ	2.56	0.41
1:F:186:VAL:HG11	2:G:135:LEU:HD22	2.02	0.41
3:C:18:VAL:HG23	3:C:86:LEU:HD11	2.02	0.41
3:H:18:VAL:HG23	3:H:86:LEU:HD11	2.03	0.41
4:D:133:CYS:HB2	4:D:147:TRP:CH2	2.56	0.41
4:D:8:PRO:HG2	4:D:11:LEU:HG	2.03	0.40
4:D:3:GLN:N	4:D:26:SER:OG	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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%)	180 (96%)	7 (4%)	30	57
1	F	187/200 (94%)	180 (96%)	7 (4%)	30	57
2	B	185/187 (99%)	179 (97%)	6 (3%)	34	60
2	G	186/187 (100%)	180 (97%)	6 (3%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	185/198 (93%)	180 (97%)	5 (3%)	39	64
3	H	184/198 (93%)	176 (96%)	8 (4%)	26	53
4	D	185/187 (99%)	182 (98%)	3 (2%)	55	72
4	I	185/187 (99%)	182 (98%)	3 (2%)	55	72
5	E	102/117 (87%)	97 (95%)	5 (5%)	22	50
5	J	101/117 (86%)	100 (99%)	1 (1%)	68	77
All	All	1687/1778 (95%)	1636 (97%)	51 (3%)	36	62

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	35	HIS
1	A	78	THR
1	A	98	ARG
1	A	121	THR
1	A	125	SER
1	A	198	THR
2	B	20	THR
2	B	58	ILE
2	B	80	SER
2	B	102	THR
2	B	104	LEU
2	B	203	SER
3	C	28	ASN
3	C	29	ILE
3	C	78	THR
3	C	81	MET
3	C	125	SER
4	D	7	SER
4	D	73	THR
4	D	89	GLN
5	E	77	SER
5	E	95	ILE
5	E	125	GLU
5	E	151	GLU
5	E	169	ASP
1	F	29	ILE
1	F	35	HIS
1	F	83	LEU

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Mol	Chain	Res	Type
1	F	98	ARG
1	F	155	VAL
1	F	201	CYS
1	F	204	ASN
2	G	29	ILE
2	G	58	ILE
2	G	80	SER
2	G	104	LEU
2	G	136	LEU
2	G	171	SER
3	H	28	ASN
3	H	29	ILE
3	H	78	THR
3	H	81	MET
3	H	121	THR
3	H	125	SER
3	H	198	THR
3	H	204	ASN
4	I	69	ASP
4	I	73	THR
4	I	89	GLN
5	J	169	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	205	HIS
2	B	53	GLN
2	B	92	ASN
2	B	100	GLN
4	D	88	GLN
4	D	159	GLN
5	E	138	GLN
1	F	110	GLN
1	F	169	HIS
2	G	100	GLN
2	G	160	GLN
3	H	33	HIS
3	H	205	HIS
4	I	36	GLN
4	I	91	HIS

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Mol	Chain	Res	Type
4	I	123	GLN
4	I	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	0.64	0	7,12,14	1.14	1 (14%)
4	SEP	D	55	4	8,9,10	0.83	0	7,12,14	1.20	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
4	SEP	I	55	4	-	2/6/8/10	-
4	SEP	D	55	4	-	3/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	55	SEP	OG-P-O1P	-2.08	100.81	106.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	55	SEP	C-CA-CB-OG
4	I	55	SEP	N-CA-CB-OG
4	I	55	SEP	C-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 oligosaccharides 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 ⓘ

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, 95th 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 ²)	Q < 0.9
1	A	219/232 (94%)	0.34	12 (5%)	30	16	51, 94, 149, 231	17 (7%)
1	F	219/232 (94%)	0.38	9 (4%)	41	22	48, 106, 170, 226	20 (9%)
2	B	212/214 (99%)	0.04	3 (1%)	73	51	47, 77, 144, 209	14 (6%)
2	G	213/214 (99%)	0.07	2 (0%)	81	61	51, 89, 163, 194	17 (7%)
3	C	219/232 (94%)	0.34	5 (2%)	61	38	58, 108, 162, 237	19 (8%)
3	H	218/232 (93%)	1.37	45 (20%)	2	1	105, 237, 535, 689	3 (1%)
4	D	209/213 (98%)	0.27	6 (2%)	53	31	45, 103, 168, 188	20 (9%)
4	I	209/213 (98%)	0.90	17 (8%)	18	9	85, 211, 384, 608	5 (2%)
5	E	112/131 (85%)	-0.02	1 (0%)	81	61	47, 70, 134, 198	5 (4%)
5	J	110/131 (83%)	0.02	1 (0%)	81	61	51, 75, 130, 154	9 (8%)
All	All	1940/2044 (94%)	0.41	101 (5%)	33	16	45, 106, 321, 689	129 (6%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	112	THR	4.5
3	C	219	LYS	4.0
3	H	114	VAL	4.0
3	H	186	VAL	4.0
3	H	108	TRP	4.0
3	H	4	LEU	3.9
1	A	140	THR	3.8
3	H	96	CYS	3.7
3	H	100	GLY	3.6
3	H	113	LEU	3.5
2	B	180	THR	3.4
4	I	167	SER	3.2
3	H	187	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	H	30	LYS	3.1
3	H	184	SER	3.1
4	I	85	TYR	3.1
3	H	22	CYS	3.0
4	I	160	GLU	3.0
3	H	2	VAL	2.9
1	F	188	THR	2.9
3	H	94	TYR	2.9
3	H	115	THR	2.8
4	I	180	LEU	2.8
3	H	107	TYR	2.8
3	H	105	PHE	2.8
1	F	187	VAL	2.8
4	D	130	SER	2.8
4	I	161	SER	2.8
4	I	162	VAL	2.8
1	A	139	GLY	2.8
3	H	26	GLY	2.8
5	J	140	GLU	2.8
1	F	159	TRP	2.7
1	A	133	SER	2.7
4	I	97	PHE	2.7
1	A	138	GLY	2.7
4	I	135	LEU	2.7
4	I	186	GLU	2.7
1	F	146	LEU	2.6
3	H	29	ILE	2.6
1	A	195	GLY	2.6
3	H	34	MET	2.6
2	B	135	LEU	2.6
2	B	179	LEU	2.6
3	H	106	ALA	2.6
3	H	125	SER	2.5
3	H	144	GLY	2.5
5	E	140	GLU	2.5
3	H	53	PRO	2.5
1	F	209	ASN	2.5
3	H	70	ILE	2.5
3	H	27	PHE	2.5
1	A	184	SER	2.5
4	D	208	PHE	2.5
3	C	96	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	188	THR	2.4
4	I	124	LEU	2.4
3	H	32	THR	2.4
3	H	18	VAL	2.4
3	H	98	ARG	2.4
4	D	176	SER	2.4
1	A	131	PRO	2.4
3	H	93	VAL	2.4
3	H	8	GLY	2.3
3	H	9	ALA	2.3
1	A	143	LEU	2.3
3	C	135	SER	2.3
3	H	56	GLY	2.3
4	I	99	GLY	2.3
3	H	102	ASN	2.3
3	H	157	VAL	2.3
1	F	186	VAL	2.3
4	D	190	VAL	2.3
4	I	132	VAL	2.3
3	C	218	PRO	2.2
1	F	184	SER	2.2
3	H	162	GLY	2.2
4	I	79	PRO	2.2
4	I	39	PRO	2.2
2	G	192	TYR	2.2
3	C	216	VAL	2.2
3	H	185	SER	2.2
3	H	72	VAL	2.2
3	H	45	LEU	2.2
1	A	66	GLY	2.2
3	H	51	ILE	2.1
4	I	159	GLN	2.1
2	G	202	SER	2.1
1	F	204	ASN	2.1
4	I	29	VAL	2.1
3	H	203	VAL	2.1
4	D	122	GLU	2.1
1	A	177	SER	2.1
4	I	145	VAL	2.1
3	H	109	GLY	2.1
4	D	145	VAL	2.0
3	H	101	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	218	PRO	2.0
3	H	97	ALA	2.0
1	F	219	LYS	2.0
1	A	186	VAL	2.0

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, 95th 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(Å ²)	Q<0.9
4	SEP	I	55	10/11	0.86	0.12	106,114,124,134	0
4	SEP	D	55	10/11	0.90	0.09	53,65,75,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.