



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9D96 / pdb_00009d96
Title : KIR3DL - HLA complex
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Deposited on : 2024-08-21
Resolution : 2.40 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

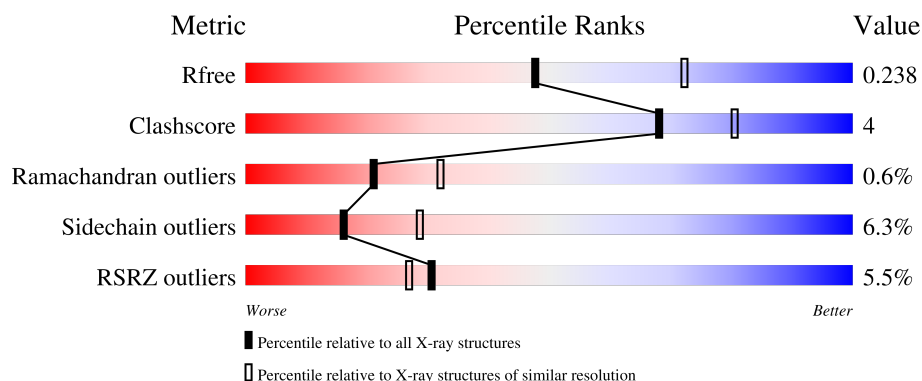
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	276	3% 88% 11% .
2	B	100	3% 85% 14% .
3	C	10	50% 70% 10% 20%
4	G	301	7% 81% 15% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5500 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2248	1401	412	428	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			830	529	140	157	4			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Epstein-Barr nuclear antigen 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			80	52	12	16			

- Molecule 4 is a protein called Killer cell immunoglobulin-like receptor 3DL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	289	Total	C	N	O	S	0	0	0
			2209	1405	400	391	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP P43629
G	0	SER	-	expression tag	UNP P43629
G	1	HIS	-	expression tag	UNP P43629

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

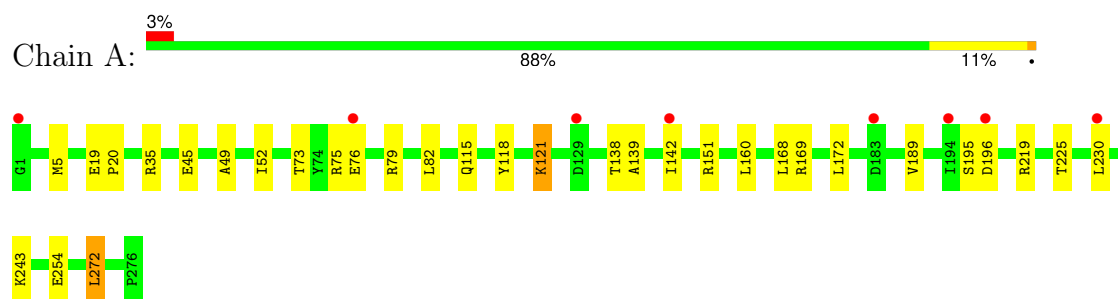
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	18	Total	O	0	0
			18	18		
6	C	2	Total	O	0	0
			2	2		
6	G	26	Total	O	0	0
			26	26		

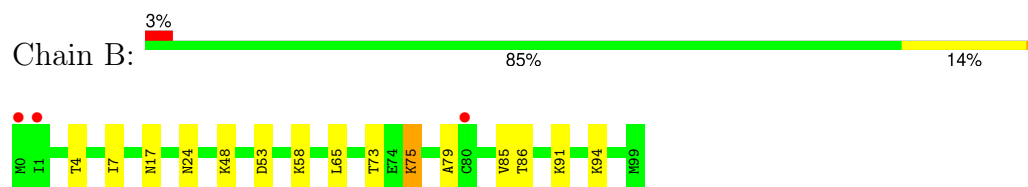
3 Residue-property plots [i](#)

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.

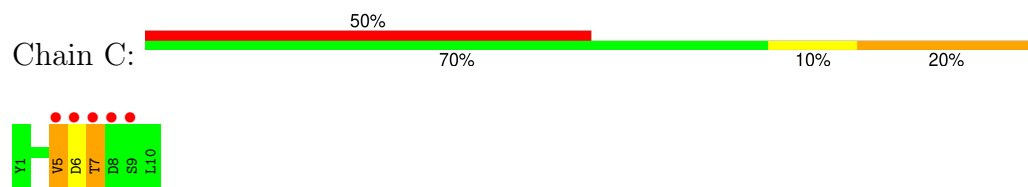
- Molecule 1: MHC class I antigen



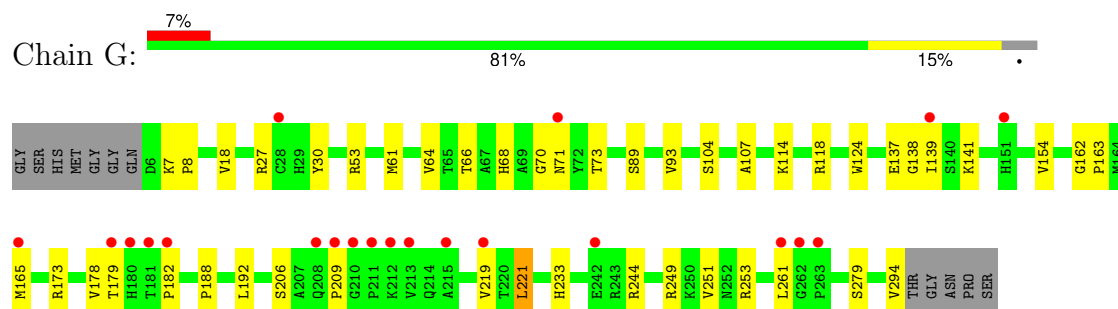
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Epstein-Barr nuclear antigen 2



- Molecule 4: Killer cell immunoglobulin-like receptor 3DL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.35Å 60.59Å 63.29Å 95.06° 95.61° 106.37°	Depositor
Resolution (Å)	41.97 – 2.40 41.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.97-2.40) 97.8 (41.97-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.201 , 0.238 0.201 , 0.238	Depositor DCC
R_{free} test set	1195 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5500	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/2311	0.27	0/3145
2	B	0.09	0/853	0.27	0/1154
3	C	0.22	0/81	0.55	0/109
4	G	0.12	0/2283	0.33	1/3111 (0.0%)
All	All	0.11	0/5528	0.30	1/7519 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	70	GLY	CA-C-O	-5.34	118.00	122.33

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	2248	0	2108	12	0
2	B	830	0	792	6	0
3	C	80	0	78	4	0
4	G	2209	0	2099	18	0
5	G	42	0	39	0	0
6	A	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	0	0	0
6	C	2	0	0	0	0
6	G	26	0	0	0	0
All	All	5500	0	5116	38	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 4.

All (38) 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:5:MET:HG3	1:A:168:LEU:HD13	1.67	0.76
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.70	0.74
2:B:4:THR:HA	2:B:86:THR:HG21	1.71	0.71
4:G:118:ARG:HG2	4:G:162:GLY:HA3	1.73	0.69
1:A:20:PRO:HB2	1:A:75:ARG:HG2	1.80	0.63
4:G:8:PRO:HG2	4:G:89:SER:HB3	1.80	0.62
4:G:8:PRO:HB3	4:G:30:TYR:HB2	1.85	0.58
4:G:107:ALA:HB2	4:G:192:LEU:HD21	1.88	0.55
4:G:173:ARG:HH11	4:G:188:PRO:HB2	1.71	0.54
1:A:73:THR:O	1:A:76:GLU:HG3	2.06	0.54
3:C:5:VAL:HG13	3:C:6:ASP:H	1.73	0.52
4:G:71:ASN:HB3	4:G:93:VAL:HG22	1.93	0.51
2:B:79:ALA:HB2	2:B:94:LYS:HD3	1.92	0.50
4:G:61:MET:HE2	4:G:68:HIS:CD2	2.46	0.49
4:G:18:VAL:HG21	4:G:64:VAL:HG21	1.96	0.47
1:A:189:VAL:HG23	1:A:272:LEU:HD23	1.97	0.47
4:G:138:GLY:HA3	4:G:141:LYS:NZ	2.30	0.46
4:G:249:ARG:HH21	4:G:253:ARG:HB3	1.80	0.46
2:B:75:LYS:H	2:B:75:LYS:HG3	1.61	0.46
4:G:221:LEU:HG	4:G:261:LEU:HD21	1.97	0.46
4:G:138:GLY:HA3	4:G:141:LYS:HZ3	1.82	0.44
1:A:19:GLU:H	1:A:19:GLU:CD	2.24	0.44
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.18	0.44
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.99	0.43
2:B:7:ILE:HD12	2:B:91:LYS:HE2	2.00	0.43
3:C:5:VAL:O	3:C:7:THR:N	2.50	0.43
4:G:233:HIS:CE1	4:G:244:ARG:HD2	2.54	0.43
4:G:104:SER:HB2	4:G:124:TRP:CE2	2.54	0.43
1:A:139:ALA:O	1:A:142:ILE:HG12	2.19	0.43
3:C:5:VAL:O	3:C:7:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:OG	1:A:196:ASP:N	2.51	0.42
3:C:5:VAL:HG13	3:C:6:ASP:N	2.33	0.42
1:A:118:TYR:O	1:A:121:LYS:HG3	2.20	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.41
4:G:7:LYS:HG3	4:G:89:SER:HA	2.03	0.41
4:G:162:GLY:HA2	4:G:163:PRO:C	2.46	0.41
1:A:73:THR:OG1	4:G:165:MET:HE1	2.20	0.41
4:G:71:ASN:HA	4:G:93:VAL:HA	2.04	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	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
4	G	287/301 (95%)	273 (95%)	11 (4%)	3 (1%)	12	20
All	All	667/687 (97%)	643 (96%)	20 (3%)	4 (1%)	21	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	209	PRO
3	C	5	VAL
4	G	137	GLU
4	G	182	PRO

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	234/237 (99%)	220 (94%)	14 (6%)	17	31
2	B	93/95 (98%)	87 (94%)	6 (6%)	15	27
3	C	9/10 (90%)	8 (89%)	1 (11%)	6	9
4	G	235/257 (91%)	220 (94%)	15 (6%)	16	28
All	All	571/599 (95%)	535 (94%)	36 (6%)	16	29

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	79	ARG
1	A	82	LEU
1	A	115	GLN
1	A	121	LYS
1	A	138	THR
1	A	151	ARG
1	A	160	LEU
1	A	169	ARG
1	A	172	LEU
1	A	219	ARG
1	A	225	THR
1	A	254	GLU
1	A	272	LEU
2	B	17	ASN
2	B	48	LYS
2	B	58	LYS
2	B	73	THR
2	B	75	LYS
2	B	85	VAL
3	C	7	THR
4	G	27	ARG
4	G	53	ARG
4	G	66	THR

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Mol	Chain	Res	Type
4	G	73	THR
4	G	114	LYS
4	G	139	ILE
4	G	154	VAL
4	G	178	VAL
4	G	179	THR
4	G	206	SER
4	G	219	VAL
4	G	221	LEU
4	G	251	VAL
4	G	279	SER
4	G	294	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	180	GLN
1	A	188	HIS
1	A	218	GLN
2	B	13	HIS
2	B	89	GLN
4	G	99	ASN
4	G	108	HIS
4	G	256	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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
5	NAG	G	303	4	14,14,15	0.98	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	G	302	4	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	G	301	4	14,14,15	0.35	0	17,19,21	0.56	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
5	NAG	G	303	4	-	4/6/23/26	0/1/1/1
5	NAG	G	302	4	-	2/6/23/26	0/1/1/1
5	NAG	G	301	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	303	NAG	O5-C1	3.10	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	303	NAG	C1-O5-C5	4.10	117.69	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	302	NAG	O5-C5-C6-O6
5	G	303	NAG	O5-C5-C6-O6
5	G	301	NAG	O5-C5-C6-O6
5	G	301	NAG	C4-C5-C6-O6
5	G	302	NAG	C4-C5-C6-O6
5	G	303	NAG	C8-C7-N2-C2
5	G	303	NAG	O7-C7-N2-C2

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, 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	276/276 (100%)	0.34	8 (2%)	53	50	27, 43, 71, 103	1 (0%)
2	B	100/100 (100%)	0.40	3 (3%)	52	48	30, 44, 78, 90	0
3	C	10/10 (100%)	2.56	5 (50%)	0	0	42, 65, 98, 119	0
4	G	289/301 (96%)	0.65	21 (7%)	21	17	30, 52, 101, 113	0
All	All	675/687 (98%)	0.51	37 (5%)	30	27	27, 47, 86, 119	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	THR	5.1
3	C	6	ASP	4.9
1	A	76	GLU	4.4
1	A	1	GLY	3.5
2	B	0	MET	3.2
4	G	213	VAL	3.1
3	C	8	ASP	3.1
4	G	262	GLY	3.1
3	C	5	VAL	3.0
4	G	209	PRO	3.0
4	G	179	THR	2.9
4	G	263	PRO	2.7
3	C	9	SER	2.7
4	G	211	PRO	2.6
4	G	208	GLN	2.6
4	G	181	THR	2.5
4	G	151	HIS	2.5
1	A	142	ILE	2.5
4	G	210	GLY	2.5
4	G	219	VAL	2.5
4	G	180	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	80	CYS	2.4
4	G	242	GLU	2.4
1	A	196	ASP	2.3
4	G	139	ILE	2.3
4	G	165	MET	2.3
1	A	230	LEU	2.3
4	G	212	LYS	2.3
4	G	28	CYS	2.3
1	A	194	ILE	2.2
4	G	215	ALA	2.2
2	B	1	ILE	2.1
4	G	261	LEU	2.1
4	G	182	PRO	2.1
1	A	129	ASP	2.0
1	A	183	ASP	2.0
4	G	71	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 oligosaccharides 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, 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
5	NAG	G	302	14/15	0.65	0.17	71,82,97,98	0
5	NAG	G	301	14/15	0.72	0.14	67,88,102,102	0
5	NAG	G	303	14/15	0.77	0.16	75,87,96,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.