



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:46 PM UTC

PDB ID : 3C8J / pdb_00003c8j
Title : The crystal structure of natural killer cell receptor Ly49C
Authors : Deng, L.; Mariuzza, R.A.
Deposited on : 2008-02-12
Resolution : 2.60 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
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

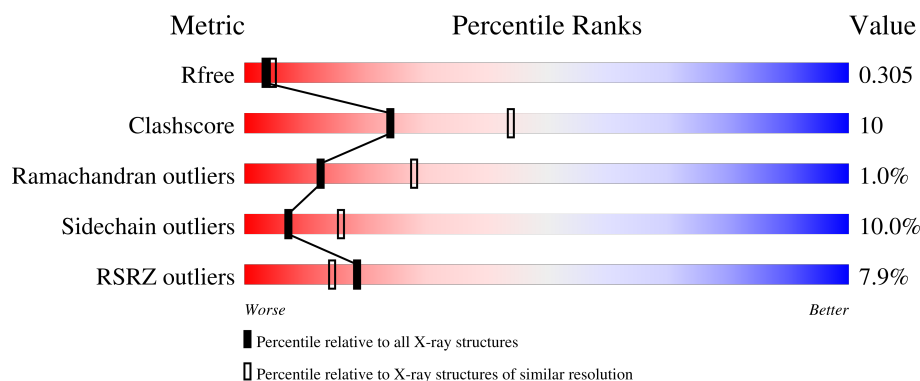
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	203	 5% 47% 12% • 37%
1	B	203	 6% 46% 13% •• 38%
1	C	203	 5% 43% 17% • 38%
1	D	203	 3% 41% 19% • 36%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4346 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 Natural killer cell receptor Ly49C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1054	687	175	181	11			
1	B	126	Total	C	N	O	S	0	0	0
			1050	684	174	181	11			
1	C	126	Total	C	N	O	S	0	0	0
			1050	684	174	181	11			
1	D	130	Total	C	N	O	S	0	0	0
			1082	701	181	189	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP Q61198
A	62	SER	VAL	SEE REMARK 999	UNP Q61198
A	74	THR	ILE	SEE REMARK 999	UNP Q61198
A	?	-	HIS	SEE REMARK 999	UNP Q61198
A	116	GLY	ARG	engineered mutation	UNP Q61198
A	119	HIS	-	SEE REMARK 999	UNP Q61198
A	171	GLY	SER	engineered mutation	UNP Q61198
A	193	GLY	GLU	engineered mutation	UNP Q61198
A	223	LYS	ARG	engineered mutation	UNP Q61198
B	60	MET	-	initiating methionine	UNP Q61198
B	62	SER	VAL	SEE REMARK 999	UNP Q61198
B	74	THR	ILE	SEE REMARK 999	UNP Q61198
B	?	-	HIS	variant	UNP Q61198
B	116	GLY	ARG	engineered mutation	UNP Q61198
B	119	HIS	-	SEE REMARK 999	UNP Q61198
B	171	GLY	SER	engineered mutation	UNP Q61198
B	193	GLY	GLU	engineered mutation	UNP Q61198
B	223	LYS	ARG	engineered mutation	UNP Q61198
C	60	MET	-	initiating methionine	UNP Q61198
C	62	SER	VAL	SEE REMARK 999	UNP Q61198
C	74	THR	ILE	SEE REMARK 999	UNP Q61198

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	HIS	SEE REMARK 999	UNP Q61198
C	116	GLY	ARG	engineered mutation	UNP Q61198
C	119	HIS	-	SEE REMARK 999	UNP Q61198
C	171	GLY	SER	engineered mutation	UNP Q61198
C	193	GLY	GLU	engineered mutation	UNP Q61198
C	223	LYS	ARG	engineered mutation	UNP Q61198
D	60	MET	-	initiating methionine	UNP Q61198
D	62	SER	VAL	SEE REMARK 999	UNP Q61198
D	74	THR	ILE	SEE REMARK 999	UNP Q61198
D	?	-	HIS	SEE REMARK 999	UNP Q61198
D	116	GLY	ARG	engineered mutation	UNP Q61198
D	119	HIS	-	SEE REMARK 999	UNP Q61198
D	171	GLY	SER	engineered mutation	UNP Q61198
D	193	GLY	GLU	engineered mutation	UNP Q61198
D	223	LYS	ARG	engineered mutation	UNP Q61198

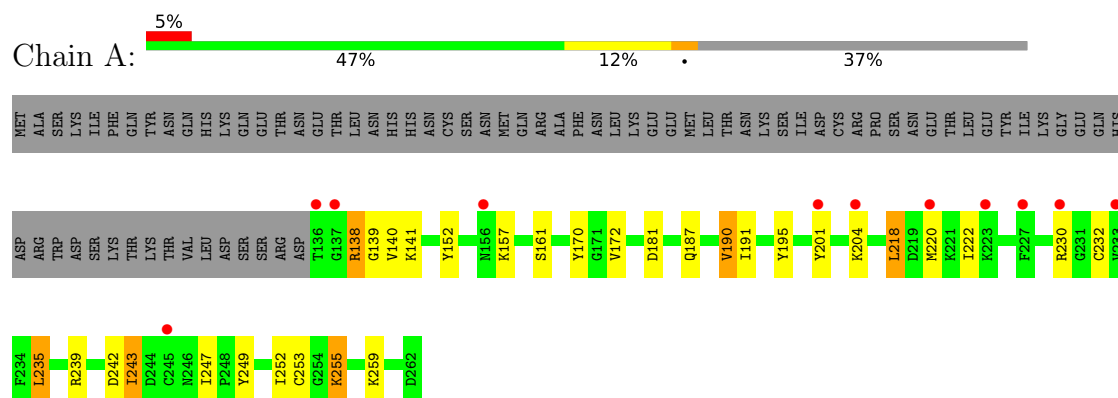
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	44	Total O 44 44	0	0
2	C	12	Total O 12 12	0	0
2	D	34	Total O 34 34	0	0

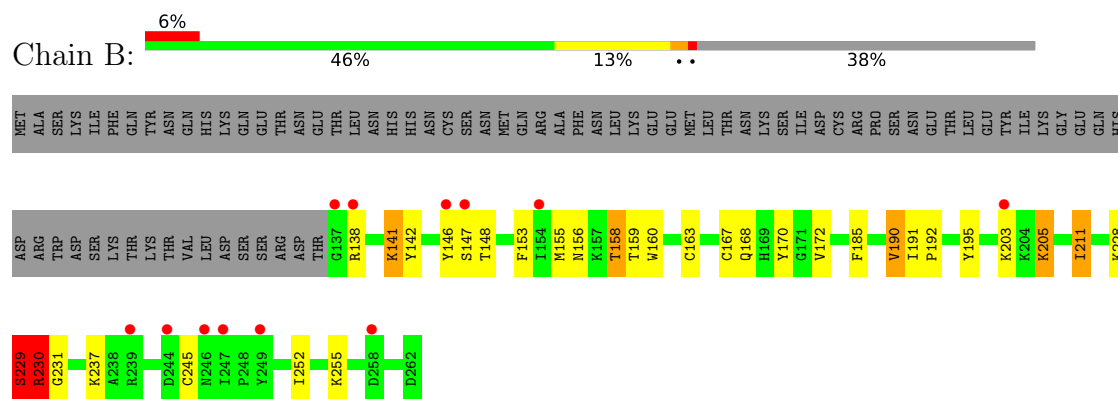
3 Residue-property plots [i](#)

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.

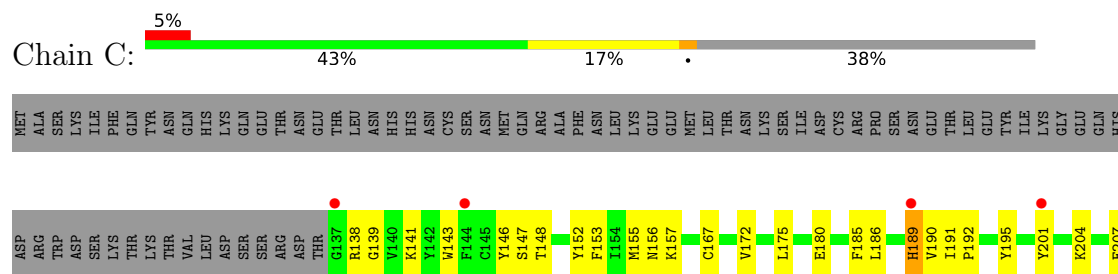
• Molecule 1: Natural killer cell receptor Ly49C

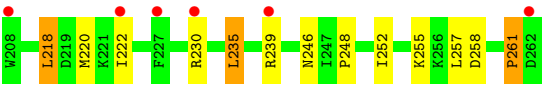


• Molecule 1: Natural killer cell receptor Ly49C

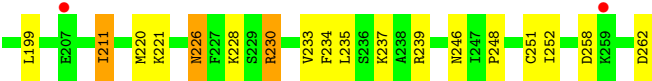
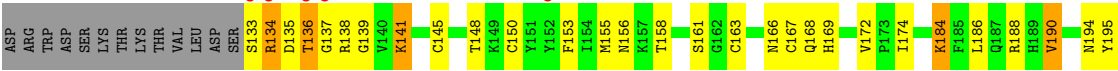


• Molecule 1: Natural killer cell receptor Ly49C





● Molecule 1: Natural killer cell receptor Ly49C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.10Å 94.89Å 104.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-2.60) 93.4 (30.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.198 , 0.263 0.259 , 0.305	Depositor DCC
R_{free} test set	1276 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4346	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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](#)

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	0/1085	0.90	1/1457 (0.1%)
1	B	0.83	0/1081	1.08	1/1450 (0.1%)
1	C	0.74	2/1081 (0.2%)	0.89	2/1450 (0.1%)
1	D	0.66	0/1113	0.98	4/1493 (0.3%)
All	All	0.72	2/4360 (0.0%)	0.97	8/5850 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	GLU	CD-OE2	11.30	1.46	1.25
1	C	207	GLU	CD-OE1	9.86	1.44	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	THR	CA-C-O	8.63	130.13	119.95
1	D	148	THR	O-C-N	-7.79	112.68	122.26
1	C	148	THR	CA-C-O	7.67	130.04	120.15
1	C	148	THR	O-C-N	-6.47	113.84	122.19
1	B	148	THR	CA-C-O	6.24	128.10	120.55
1	D	230	ARG	N-CA-C	-5.69	105.25	113.21
1	A	139	GLY	N-CA-C	5.65	118.63	111.85
1	D	239	ARG	N-CA-C	5.31	115.55	108.38

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	1054	0	1038	14	0
1	B	1050	0	1036	22	0
1	C	1050	0	1036	23	1
1	D	1082	0	1065	29	1
2	A	20	0	0	1	0
2	B	44	0	0	2	0
2	C	12	0	0	1	0
2	D	34	0	0	6	0
All	All	4346	0	4175	84	1

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 10.

All (84) 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:D:135:ASP:HA	2:D:297:HOH:O	1.48	1.14
1:D:138:ARG:HB3	1:D:156:ASN:HD21	1.24	1.01
1:D:136:THR:OG1	1:D:137:GLY:N	1.96	0.91
1:C:155:MET:HE1	1:C:195:TYR:HE2	1.37	0.88
1:D:190:VAL:O	1:D:237:LYS:HE2	1.74	0.88
1:C:155:MET:HE1	1:C:195:TYR:CE2	2.15	0.82
1:B:153:PHE:HB3	1:B:155:MET:HE2	1.61	0.80
1:C:139:GLY:H	1:C:156:ASN:HD21	1.33	0.77
1:B:205:LYS:HB2	2:B:275:HOH:O	1.86	0.76
1:D:138:ARG:HB3	1:D:156:ASN:ND2	2.01	0.74
1:D:136:THR:HG1	1:D:137:GLY:H	1.37	0.70
1:B:190:VAL:O	1:B:237:LYS:HE2	1.92	0.69
1:D:188:ARG:HD3	2:D:319:HOH:O	1.94	0.67
1:D:251:CYS:HB2	2:D:300:HOH:O	1.95	0.66
1:D:188:ARG:CD	2:D:319:HOH:O	2.45	0.64
1:B:158:THR:HG23	1:B:159:THR:O	1.98	0.63
1:C:172:VAL:HG13	1:C:255:LYS:HB2	1.81	0.62
1:D:167:CYS:HB3	1:D:172:VAL:O	2.00	0.61
1:C:167:CYS:HB3	1:C:172:VAL:O	2.00	0.61
1:B:138:ARG:HH21	1:D:184:LYS:HD2	1.65	0.60
1:B:142:TYR:HE2	1:B:155:MET:HE3	1.68	0.58
1:C:139:GLY:H	1:C:156:ASN:ND2	2.01	0.58
1:C:153:PHE:CE1	1:C:189:HIS:HE1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LYS:O	1:B:229:SER:HB3	2.05	0.57
1:C:139:GLY:N	1:C:156:ASN:HD21	1.99	0.57
1:A:195:TYR:HB3	1:A:252:ILE:HG13	1.89	0.55
1:B:167:CYS:HB3	1:B:172:VAL:O	2.07	0.55
1:D:133:SER:O	1:D:134:ARG:HG3	2.07	0.54
1:D:166:ASN:O	1:D:169:HIS:HB3	2.08	0.54
1:A:141:LYS:HE2	1:A:170:TYR:CZ	2.44	0.53
1:C:201:TYR:CE2	1:C:230:ARG:HG2	2.45	0.52
1:A:235:LEU:HD12	1:A:235:LEU:C	2.35	0.52
1:C:143:TRP:HB3	1:C:152:TYR:HD1	1.74	0.52
1:A:152:TYR:HB2	1:A:253:CYS:HB2	1.93	0.51
1:B:228:LYS:O	1:B:229:SER:CB	2.56	0.51
1:D:174:ILE:HG22	1:D:211:ILE:HD12	1.93	0.51
1:B:153:PHE:HB3	1:B:155:MET:CE	2.36	0.50
1:C:218:LEU:HB3	1:C:222:ILE:HD12	1.94	0.50
1:A:201:TYR:CE2	1:A:230:ARG:HG2	2.47	0.50
1:B:141:LYS:HE2	1:B:170:TYR:CZ	2.47	0.49
1:C:156:ASN:ND2	2:C:265:HOH:O	2.45	0.49
1:B:146:TYR:O	1:B:147:SER:C	2.52	0.48
1:B:191:ILE:O	1:B:192:PRO:C	2.56	0.48
1:A:218:LEU:HB3	1:A:222:ILE:HD12	1.94	0.48
1:B:172:VAL:HG13	1:B:255:LYS:HB2	1.95	0.47
1:A:181:ASP:CG	1:C:138:ARG:HD2	2.39	0.47
1:D:158:THR:O	1:D:248:PRO:HA	2.15	0.47
1:D:133:SER:C	1:D:134:ARG:HG3	2.40	0.47
1:D:139:GLY:O	1:D:141:LYS:HE2	2.15	0.46
1:D:199:LEU:HD23	1:D:233:VAL:HG21	1.97	0.46
1:D:163:CYS:HB2	2:D:300:HOH:O	2.14	0.46
1:C:146:TYR:CD1	1:C:185:PHE:CE1	3.04	0.46
1:D:186:LEU:O	1:D:190:VAL:HB	2.16	0.46
1:C:175:LEU:HD21	1:C:186:LEU:CD1	2.46	0.46
1:D:194:ASN:HB3	1:D:234:PHE:CD1	2.52	0.45
1:B:138:ARG:NH2	1:D:184:LYS:HD2	2.31	0.45
1:D:145:CYS:HA	1:D:150:CYS:HA	1.99	0.45
1:B:211:ILE:HA	2:B:276:HOH:O	2.16	0.45
1:C:191:ILE:O	1:C:192:PRO:C	2.57	0.44
1:B:231:GLY:HA2	1:B:245:CYS:SG	2.57	0.44
1:A:187:GLN:HE22	1:A:239:ARG:HA	1.81	0.44
1:B:230:ARG:HD2	1:B:230:ARG:C	2.42	0.44
1:C:143:TRP:HB3	1:C:152:TYR:CD1	2.52	0.44
1:D:220:MET:HA	1:D:220:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HA	1:A:249:TYR:O	2.17	0.44
1:C:146:TYR:O	1:C:147:SER:C	2.59	0.44
1:D:153:PHE:CE2	1:D:190:VAL:HG23	2.53	0.44
1:C:235:LEU:C	1:C:235:LEU:HD12	2.43	0.43
1:A:232:CYS:O	1:A:242:ASP:HA	2.18	0.43
1:A:243:ILE:HG12	1:A:247:ILE:HD12	1.99	0.43
1:B:153:PHE:CB	1:B:155:MET:HE2	2.40	0.43
1:B:195:TYR:HB3	1:B:252:ILE:HG13	1.99	0.43
1:D:226:ASN:O	1:D:228:LYS:HG2	2.18	0.43
1:A:172:VAL:HG13	1:A:255:LYS:HB3	2.00	0.43
1:B:146:TYR:CD1	1:B:185:PHE:CE1	3.06	0.43
1:C:175:LEU:HD21	1:C:186:LEU:HD13	2.01	0.42
1:C:261:PRO:HG2	1:D:150:CYS:SG	2.60	0.42
1:A:140:VAL:HA	2:A:263:HOH:O	2.19	0.42
1:A:190:VAL:HG13	1:A:191:ILE:O	2.20	0.42
1:B:160:TRP:O	1:B:163:CYS:HB3	2.20	0.42
1:C:195:TYR:HB3	1:C:252:ILE:HG13	2.01	0.41
1:C:157:LYS:HB3	1:C:248:PRO:HB2	2.03	0.41
1:D:195:TYR:HB3	1:D:252:ILE:HG13	2.03	0.41
1:D:184:LYS:HE2	2:D:294:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:NH2	1:D:228:LYS:O[2_875]	1.85	0.35

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	125/203 (62%)	114 (91%)	10 (8%)	1 (1%)	16 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	124/203 (61%)	117 (94%)	5 (4%)	2 (2%)	7	16
1	C	124/203 (61%)	111 (90%)	12 (10%)	1 (1%)	16	34
1	D	128/203 (63%)	116 (91%)	11 (9%)	1 (1%)	16	34
All	All	501/812 (62%)	458 (91%)	38 (8%)	5 (1%)	12	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	B	229	SER
1	B	230	ARG
1	D	134	ARG
1	C	261	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	114/188 (61%)	104 (91%)	10 (9%)	9	21
1	B	114/188 (61%)	104 (91%)	10 (9%)	9	21
1	C	114/188 (61%)	103 (90%)	11 (10%)	8	17
1	D	118/188 (63%)	103 (87%)	15 (13%)	4	9
All	All	460/752 (61%)	414 (90%)	46 (10%)	7	16

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	A	161	SER
1	A	190	VAL
1	A	204	LYS
1	A	218	LEU
1	A	220	MET

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	243	ILE
1	A	255	LYS
1	A	259	LYS
1	B	141	LYS
1	B	156	ASN
1	B	158	THR
1	B	168	GLN
1	B	190	VAL
1	B	203	LYS
1	B	205	LYS
1	B	211	ILE
1	B	229	SER
1	B	230	ARG
1	C	141	LYS
1	C	180	GLU
1	C	189	HIS
1	C	190	VAL
1	C	204	LYS
1	C	218	LEU
1	C	220	MET
1	C	235	LEU
1	C	246	ASN
1	C	257	LEU
1	C	258	ASP
1	D	136	THR
1	D	141	LYS
1	D	155	MET
1	D	161	SER
1	D	168	GLN
1	D	184	LYS
1	D	190	VAL
1	D	211	ILE
1	D	221	LYS
1	D	226	ASN
1	D	230	ARG
1	D	235	LEU
1	D	246	ASN
1	D	258	ASP
1	D	262	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	169	HIS
1	A	187	GLN
1	A	189	HIS
1	A	194	ASN
1	B	166	ASN
1	B	194	ASN
1	B	213	ASN
1	C	156	ASN
1	C	166	ASN
1	C	168	GLN
1	C	187	GLN
1	C	189	HIS
1	C	194	ASN
1	C	246	ASN
1	D	156	ASN
1	D	187	GLN
1	D	194	ASN
1	D	246	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 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 ⓘ

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	127/203 (62%)	0.82	11 (8%) 16 12	50, 59, 72, 74	0
1	B	126/203 (62%)	0.91	12 (9%) 14 10	45, 56, 69, 81	0
1	C	126/203 (62%)	1.05	10 (7%) 18 14	53, 61, 71, 73	0
1	D	130/203 (64%)	0.85	7 (5%) 31 26	54, 61, 71, 85	0
All	All	509/812 (62%)	0.90	40 (7%) 18 14	45, 60, 71, 85	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	SER	6.6
1	C	137	GLY	4.9
1	D	136	THR	4.7
1	A	136	THR	4.3
1	D	134	ARG	3.8
1	D	137	GLY	3.5
1	D	207	GLU	3.4
1	B	138	ARG	3.3
1	C	201	TYR	3.2
1	A	137	GLY	3.0
1	B	147	SER	2.9
1	B	244	ASP	2.9
1	B	203	LYS	2.8
1	C	227	PHE	2.7
1	A	204	LYS	2.7
1	C	144	PHE	2.6
1	C	189	HIS	2.5
1	B	146	TYR	2.5
1	B	137	GLY	2.5
1	B	239	ARG	2.4
1	D	152	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	230	ARG	2.4
1	C	239	ARG	2.4
1	C	208	TRP	2.4
1	A	245	CYS	2.3
1	C	230	ARG	2.3
1	A	156	ASN	2.2
1	B	246	ASN	2.2
1	A	223	LYS	2.2
1	D	259	LYS	2.2
1	B	249	TYR	2.2
1	B	247	ILE	2.2
1	C	262	ASP	2.2
1	B	154	ILE	2.1
1	B	258	ASP	2.1
1	A	227	PHE	2.1
1	A	201	TYR	2.1
1	C	222	ILE	2.0
1	A	233	VAL	2.0
1	A	220	MET	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.