



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2022 – 10:14 PM JST

PDB ID : 7DUU
Title : Crystal structure of HLA molecule with an KIR receptor
Authors : Yang, Y.; Yin, L.
Deposited on : 2021-01-11
Resolution : 2.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.26
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) : 2.26

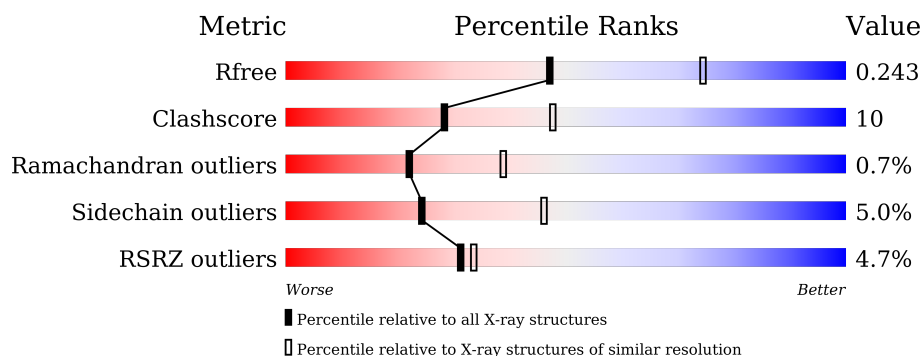
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	273	<div> <div> <div>0%</div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
2	B	100	<div> <div>2%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
3	C	9	<div> <div>44%</div> <div>56%</div> </div>
4	D	200	<div> <div>12%</div> <div>72%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4791 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	273	Total	C	N	O	S	0	0	0
			2241	1397	407	429	8			

- 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
			836	533	141	158	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 LEU-ASN-PRO-SER-VAL-ALA-ALA-THR-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			62	39	10	13			

- Molecule 4 is a protein called Killer cell immunoglobulin-like receptor 2DS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	196	Total	C	N	O	S	0	0	0
			1525	961	265	292	7			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		

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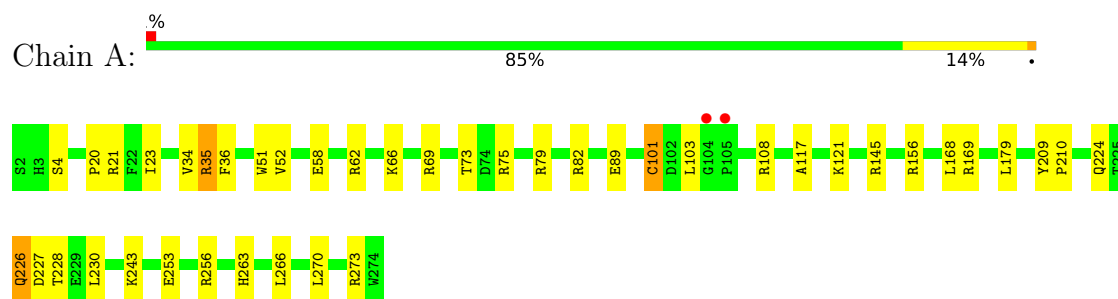
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	28	Total 28	O 28	0	0
5	C	3	Total 3	O 3	0	0
5	D	30	Total 30	O 30	0	0

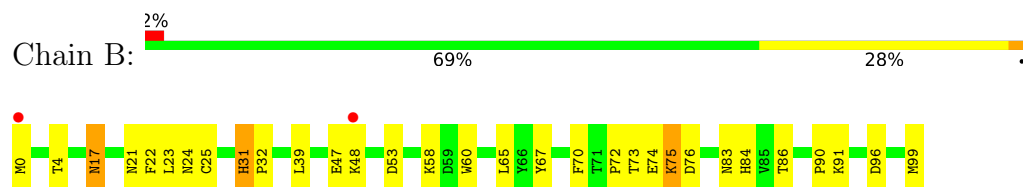
3 Residue-property plots

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.

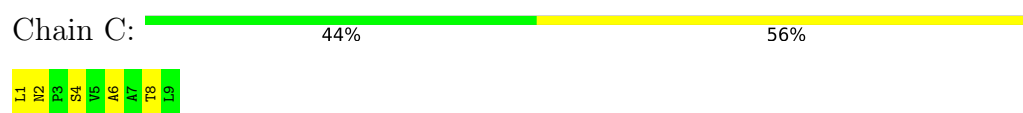
• Molecule 1: MHC class I antigen



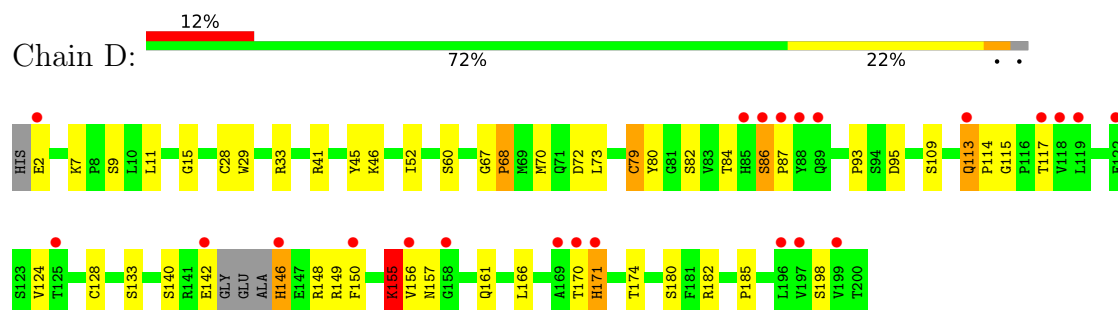
• Molecule 2: Beta-2-microglobulin



• Molecule 3: LEU-ASN-PRO-SER-VAL-ALA-ALA-THR-LEU



• Molecule 4: Killer cell immunoglobulin-like receptor 2DS2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.06Å 153.96Å 177.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.39 – 2.51 44.39 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.39-2.51) 99.3 (44.39-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.246 0.203 , 0.243	Depositor DCC
R_{free} test set	1997 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	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	4791	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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

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	0.50	1/2306 (0.0%)	0.64	0/3134
2	B	0.67	0/859	0.77	2/1162 (0.2%)
3	C	0.48	0/62	0.72	0/84
4	D	0.70	3/1570 (0.2%)	0.79	1/2131 (0.0%)
All	All	0.60	4/4797 (0.1%)	0.71	3/6511 (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
4	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	CYS	CB-SG	-9.23	1.66	1.82
4	D	115	GLY	C-N	7.74	1.49	1.34
4	D	15	GLY	C-N	6.92	1.47	1.34
4	D	79	CYS	CB-SG	-5.73	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	68	PRO	CA-N-CD	-10.06	97.42	111.50
2	B	31	HIS	N-CA-CB	7.51	124.11	110.60
2	B	31	HIS	CA-CB-CG	-5.43	104.37	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	67	GLY	Mainchain

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	2241	0	2078	33	0
2	B	836	0	803	25	0
3	C	62	0	68	5	0
4	D	1525	0	1451	35	0
5	A	66	0	0	2	0
5	B	28	0	0	2	0
5	C	3	0	0	0	0
5	D	30	0	0	1	0
All	All	4791	0	4400	89	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 10.

All (89) 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)
4:D:86:SER:OG	4:D:87:PRO:HD3	1.30	1.22
4:D:86:SER:CB	4:D:87:PRO:HD3	1.83	1.07
4:D:86:SER:CB	4:D:87:PRO:CD	2.40	0.99
2:B:4:THR:HG22	2:B:86:THR:OG1	1.63	0.97
4:D:86:SER:OG	4:D:87:PRO:CD	2.16	0.92
4:D:113:GLN:O	4:D:113:GLN:NE2	2.08	0.85
4:D:86:SER:HB3	4:D:87:PRO:CD	2.08	0.84
1:A:20:PRO:HD2	1:A:75:ARG:HD3	1.64	0.79
4:D:113:GLN:HB3	4:D:114:PRO:HD3	1.62	0.79
2:B:4:THR:HA	2:B:86:THR:HG21	1.69	0.73
4:D:140:SER:HB2	4:D:146:HIS:HA	1.73	0.70
1:A:66:LYS:HE3	3:C:4:SER:HA	1.76	0.68
4:D:41:ARG:NH1	4:D:45:TYR:O	2.26	0.67
4:D:86:SER:HG	4:D:87:PRO:HD3	1.55	0.66
4:D:113:GLN:HB3	4:D:114:PRO:CD	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LYS:HD3	2:B:75:LYS:H	1.61	0.65
1:A:145:ARG:NH1	4:D:133:SER:OG	2.30	0.65
1:A:82:ARG:NH2	1:A:89:GLU:OE1	2.29	0.64
1:A:266:LEU:HD22	1:A:270:LEU:HD13	1.81	0.63
4:D:86:SER:HB3	4:D:87:PRO:HD2	1.82	0.62
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.65	0.61
4:D:148:ARG:HG3	4:D:148:ARG:HH11	1.66	0.61
1:A:62:ARG:HH22	3:C:1:LEU:HD11	1.66	0.60
2:B:32:PRO:HD2	2:B:84:HIS:CE1	2.36	0.60
1:A:62:ARG:NH1	5:A:302:HOH:O	2.35	0.59
4:D:113:GLN:CB	4:D:114:PRO:HD3	2.31	0.59
4:D:117:THR:HG23	4:D:198:SER:HB2	1.83	0.59
1:A:66:LYS:HE2	3:C:2:ASN:HB2	1.83	0.59
4:D:156:VAL:O	4:D:156:VAL:HG13	2.02	0.58
4:D:114:PRO:HD2	4:D:124:VAL:HG23	1.85	0.57
2:B:32:PRO:HD2	2:B:84:HIS:HE1	1.70	0.57
1:A:58:GLU:O	1:A:62:ARG:HG2	2.05	0.56
1:A:21:ARG:NE	1:A:23:ILE:HD11	2.19	0.56
1:A:226:GLN:HG2	1:A:227:ASP:OD1	2.07	0.54
4:D:82:SER:OG	4:D:84:THR:O	2.25	0.53
4:D:7:LYS:NZ	4:D:95:ASP:OD1	2.40	0.53
1:A:35:ARG:HG3	2:B:53:ASP:CG	2.29	0.53
2:B:91:LYS:NZ	5:B:101:HOH:O	2.43	0.52
2:B:73:THR:HG23	2:B:76:ASP:H	1.75	0.51
1:A:69:ARG:HG3	5:A:362:HOH:O	2.10	0.50
1:A:156:ARG:NH2	3:C:6:ALA:HB1	2.27	0.50
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.94	0.50
1:A:73:THR:HG23	3:C:8:THR:HG22	1.94	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.49
1:A:224:GLN:O	1:A:228:THR:OG1	2.25	0.49
1:A:253:GLU:O	1:A:256:ARG:HG2	2.13	0.48
2:B:4:THR:HG22	2:B:86:THR:HG1	1.70	0.48
1:A:210:PRO:HD2	1:A:263:HIS:CE1	2.48	0.47
4:D:52:ILE:H	4:D:52:ILE:HD12	1.78	0.47
2:B:58:LYS:NZ	5:B:103:HOH:O	2.48	0.47
4:D:148:ARG:HH11	4:D:148:ARG:CG	2.28	0.47
2:B:84:HIS:ND1	2:B:86:THR:HG22	2.31	0.46
2:B:31:HIS:O	2:B:31:HIS:CG	2.66	0.46
1:A:108:ARG:CZ	1:A:169:ARG:HH22	2.29	0.45
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.98	0.45
2:B:17:ASN:OD1	2:B:17:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.99	0.44
1:A:35:ARG:HG2	1:A:36:PHE:N	2.33	0.44
4:D:33:ARG:HD3	5:D:309:HOH:O	2.17	0.44
4:D:124:VAL:HG13	4:D:166:LEU:HB2	2.00	0.44
2:B:31:HIS:ND1	2:B:31:HIS:C	2.71	0.44
1:A:4:SER:HB2	1:A:101:CYS:O	2.17	0.44
4:D:70:MET:HA	4:D:70:MET:HE3	2.00	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.43
4:D:80:TYR:CE2	4:D:93:PRO:HB3	2.53	0.43
2:B:84:HIS:ND1	2:B:86:THR:CG2	2.82	0.43
4:D:170:THR:OG1	4:D:171:HIS:N	2.52	0.43
2:B:96:ASP:HB3	2:B:99:MET:HE2	2.01	0.42
4:D:41:ARG:O	4:D:46:LYS:HA	2.18	0.42
4:D:155:LYS:HB3	4:D:155:LYS:HE3	1.90	0.42
1:A:51:TRP:CE3	1:A:52:VAL:HG13	2.54	0.42
4:D:114:PRO:HG2	4:D:124:VAL:HA	2.01	0.42
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.55	0.42
4:D:148:ARG:CG	4:D:148:ARG:NH1	2.82	0.42
2:B:83:ASN:ND2	2:B:90:PRO:HG3	2.35	0.42
4:D:142:GLU:HG2	4:D:174:THR:O	2.20	0.42
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.02	0.42
2:B:21:ASN:OD1	2:B:22:PHE:N	2.47	0.41
2:B:17:ASN:HA	2:B:72:PRO:O	2.20	0.41
1:A:210:PRO:HD2	1:A:263:HIS:HE1	1.84	0.41
2:B:73:THR:OG1	2:B:74:GLU:N	2.53	0.41
1:A:224:GLN:HG3	1:A:226:GLN:HE22	1.86	0.41
4:D:70:MET:H	4:D:73:LEU:HD12	1.86	0.41
1:A:79:ARG:HD2	1:A:79:ARG:HA	1.86	0.40
1:A:121:LYS:HD2	2:B:0:MET:HB3	2.03	0.40
4:D:29:TRP:HA	4:D:60:SER:O	2.21	0.40
1:A:34:VAL:HG22	1:A:35:ARG:N	2.37	0.40
4:D:9:SER:O	4:D:28:CYS:HA	2.21	0.40
1:A:103:LEU:HG	1:A:168:LEU:CD2	2.52	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	271/273 (99%)	260 (96%)	10 (4%)	1 (0%)	34	54
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	192/200 (96%)	185 (96%)	4 (2%)	3 (2%)	9	17
All	All	568/582 (98%)	546 (96%)	18 (3%)	4 (1%)	22	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	68	PRO
4	D	86	SER
4	D	155	LYS
1	A	209	TYR

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	231/231 (100%)	228 (99%)	3 (1%)	69	87
2	B	95/95 (100%)	90 (95%)	5 (5%)	22	43
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	170/172 (99%)	153 (90%)	17 (10%)	7	15
All	All	503/505 (100%)	478 (95%)	25 (5%)	24	46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	226	GLN
1	A	273	ARG
2	B	17	ASN
2	B	47	GLU
2	B	48	LYS
2	B	70	PHE
2	B	75	LYS
4	D	2	GLU
4	D	11	LEU
4	D	72	ASP
4	D	79	CYS
4	D	109	SER
4	D	113	GLN
4	D	128	CYS
4	D	146	HIS
4	D	149	ARG
4	D	150	PHE
4	D	155	LYS
4	D	157	ASN
4	D	161	GLN
4	D	171	HIS
4	D	180	SER
4	D	182	ARG
4	D	185	PRO

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

Mol	Chain	Res	Type
4	D	113	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 [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

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	273/273 (100%)	0.08	2 (0%) 87 89	29, 48, 86, 109	0
2	B	100/100 (100%)	0.25	2 (2%) 65 68	29, 52, 85, 95	0
3	C	9/9 (100%)	0.53	0 100 100	36, 44, 58, 66	0
4	D	196/200 (98%)	0.61	23 (11%) 4 4	38, 60, 98, 114	0
All	All	578/582 (99%)	0.30	27 (4%) 31 33	29, 53, 90, 114	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	156	VAL	4.9
4	D	86	SER	4.5
4	D	158	GLY	4.1
4	D	88	TYR	4.0
4	D	113	GLN	3.9
1	A	104	GLY	3.8
4	D	87	PRO	3.7
1	A	105	PRO	3.6
2	B	0	MET	3.5
4	D	119	LEU	3.4
4	D	170	THR	3.1
4	D	89	GLN	3.1
4	D	146	HIS	3.0
4	D	125	THR	3.0
4	D	171	HIS	2.8
4	D	169	ALA	2.6
4	D	2	GLU	2.6
2	B	48	LYS	2.5
4	D	150	PHE	2.5
4	D	199	VAL	2.4
4	D	117	THR	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	197	VAL	2.4
4	D	196	LEU	2.3
4	D	142	GLU	2.3
4	D	118	VAL	2.0
4	D	122	GLU	2.0
4	D	85	HIS	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 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.