



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:42 PM UTC

PDB ID : 3QDM / pdb_00003qdm
Title : The complex between TCR DMF4 and human Class I MHC HLA-A2 with the bound MART-1(26-35)(A27L) decameric peptide
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2011-01-18
Resolution : 2.80 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

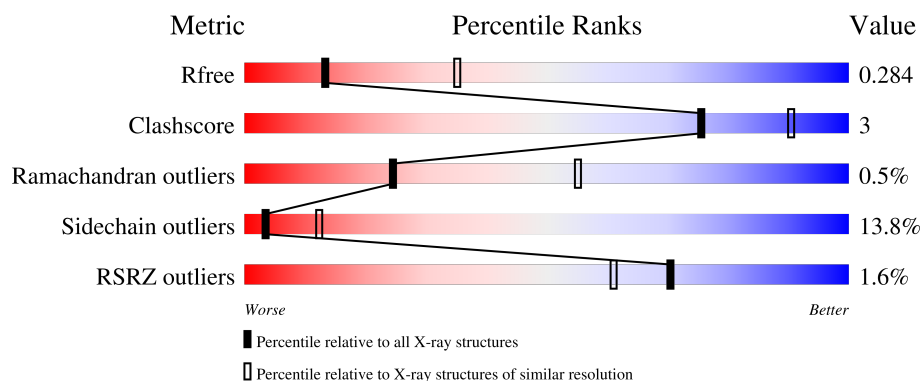
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	275	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6635 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

- 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	1	0
			843	537	141	160	5			

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 MART-1(27-35) peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	45	10	14			

- Molecule 4 is a protein called DMF4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	1	0
			1513	950	245	309	9			

- Molecule 5 is a protein called DMF4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1930	1209	339	376	6			

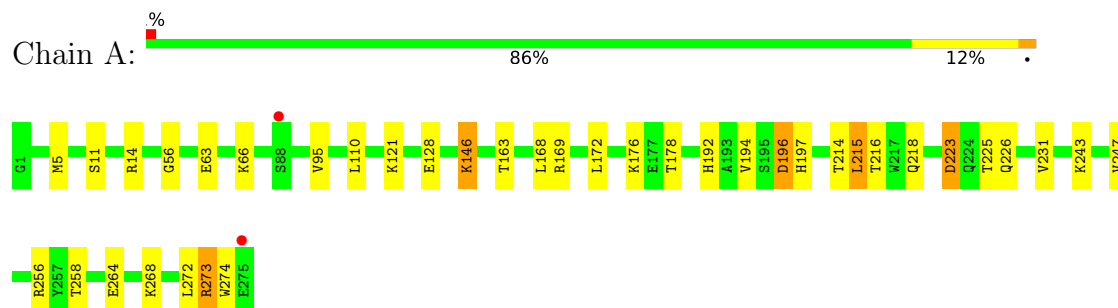
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total 14	O 14	0	0
6	B	6	Total 6	O 6	0	0
6	C	1	Total 1	O 1	0	0
6	D	7	Total 7	O 7	0	0
6	E	5	Total 5	O 5	0	0

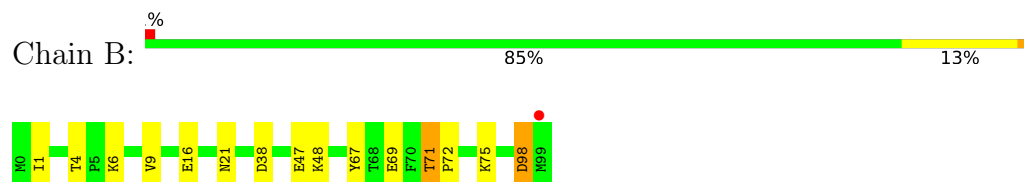
3 Residue-property plots

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.

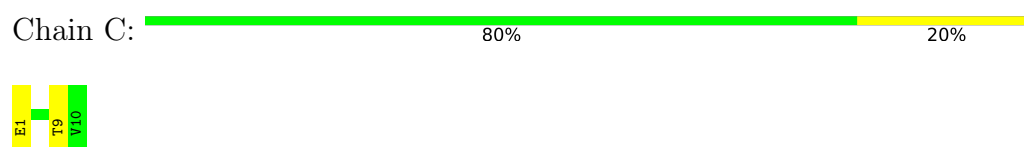
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



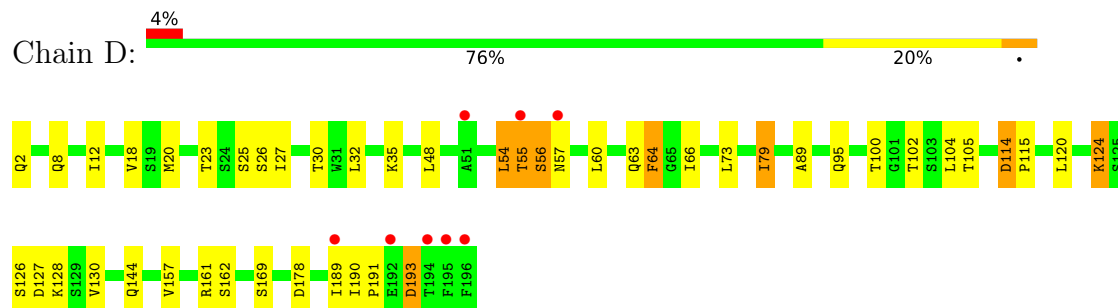
- Molecule 2: Beta-2-microglobulin



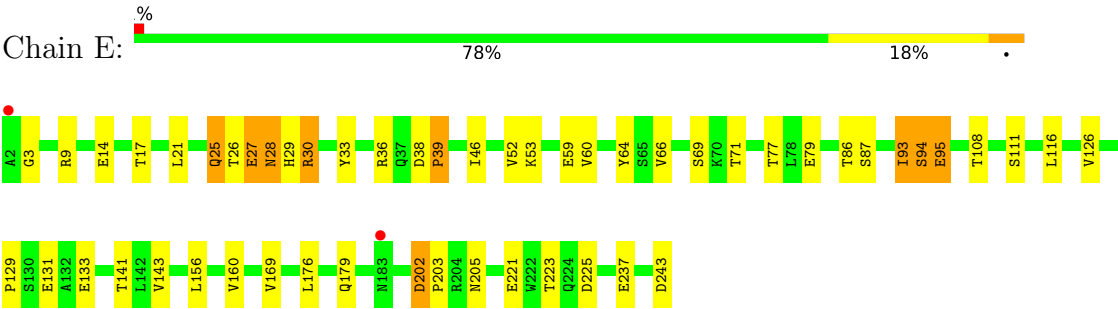
- Molecule 3: MART-1(27-35) peptide



- Molecule 4: DMF4 alpha chain



- Molecule 5: DMF4 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.01Å 69.75Å 227.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.80) 92.7 (20.00-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.284 0.213 , 0.284	Depositor DCC
R_{free} test set	1064 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6635	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 4.65% 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	0.64	0/2312	1.04	7/3137 (0.2%)
2	B	0.58	0/868	0.95	3/1169 (0.3%)
3	C	0.76	0/68	1.03	0/90
4	D	0.70	0/1549	1.12	8/2101 (0.4%)
5	E	0.66	0/1983	1.04	6/2699 (0.2%)
All	All	0.65	0/6780	1.05	24/9196 (0.3%)

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
1	A	0	1
4	D	0	2
All	All	0	3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	79	ILE	CB-CA-C	8.99	118.14	109.33
4	D	57	ASN	N-CA-C	-7.58	103.65	113.12
4	D	79	ILE	N-CA-C	-7.36	103.15	109.19
5	E	202	ASP	CA-C-N	7.13	126.83	119.56
5	E	202	ASP	C-N-CA	7.13	126.83	119.56
4	D	126	SER	N-CA-C	6.35	118.52	110.33
4	D	114	ASP	CA-C-N	6.33	126.36	119.90
4	D	114	ASP	C-N-CA	6.33	126.36	119.90
5	E	30	ARG	N-CA-C	6.19	117.63	108.60
1	A	231	VAL	CB-CA-C	-6.12	104.86	111.59
4	D	56	SER	N-CA-C	6.05	123.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	38	ASP	CA-C-N	5.94	127.27	119.84
5	E	38	ASP	C-N-CA	5.94	127.27	119.84
1	A	14	ARG	CA-C-N	5.80	127.09	119.84
1	A	14	ARG	C-N-CA	5.80	127.09	119.84
1	A	268	LYS	CA-C-N	5.59	125.54	119.78
1	A	268	LYS	C-N-CA	5.59	125.54	119.78
2	B	71	THR	CA-C-N	5.55	125.31	119.76
2	B	71	THR	C-N-CA	5.55	125.31	119.76
2	B	67	TYR	N-CA-C	5.33	117.19	108.76
5	E	237	GLU	N-CA-C	5.24	117.37	109.41
4	D	8	GLN	N-CA-C	-5.20	107.06	113.41
1	A	56	GLY	CA-C-N	5.08	125.36	119.47
1	A	56	GLY	C-N-CA	5.08	125.36	119.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	GLN	Peptide
4	D	55	THR	Peptide
4	D	56	SER	Peptide

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	2247	0	2096	10	0
2	B	843	0	812	2	0
3	C	69	0	79	0	0
4	D	1513	0	1428	10	0
5	E	1930	0	1819	20	0
6	A	14	0	0	0	0
6	B	6	0	0	0	0
6	C	1	0	0	0	0
6	D	7	0	0	0	0
6	E	5	0	0	0	0
All	All	6635	0	6234	39	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 (39) 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:196:ASP:OD1	1:A:196:ASP:N	2.14	0.77
5:E:30:ARG:NH2	5:E:95:GLU:OE2	2.23	0.72
1:A:223:ASP:OD2	1:A:223:ASP:N	2.24	0.70
4:D:178:ASP:OD1	4:D:178:ASP:N	2.41	0.53
5:E:33:TYR:HE2	5:E:94:SER:HB2	1.77	0.50
5:E:25:GLN:NE2	5:E:28:ASN:O	2.47	0.48
5:E:14:GLU:HB3	5:E:116:LEU:HG	1.95	0.48
5:E:202:ASP:OD2	5:E:205:ASN:ND2	2.46	0.48
4:D:32:LEU:HB2	4:D:89:ALA:HB3	1.96	0.47
1:A:63:GLU:OE1	1:A:66:LYS:NZ	2.38	0.47
4:D:120:LEU:HD22	5:E:129:PRO:HA	1.97	0.47
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.97	0.46
5:E:36:ARG:NH1	5:E:64:TYR:OH	2.46	0.46
4:D:48:LEU:HD13	4:D:64:PHE:HB2	1.98	0.45
5:E:86:THR:HG23	5:E:111:SER:HA	1.98	0.45
1:A:215:LEU:HD22	1:A:243:LYS:HD3	1.98	0.45
5:E:59:GLU:H	5:E:59:GLU:HG2	1.62	0.44
4:D:124:LYS:HA	4:D:124:LYS:HD2	1.49	0.44
5:E:30:ARG:HD3	5:E:93:ILE:HG23	2.00	0.44
5:E:27:GLU:H	5:E:27:GLU:HG2	1.33	0.44
5:E:30:ARG:HE	5:E:30:ARG:HB3	1.54	0.44
4:D:114:ASP:HA	4:D:115:PRO:HD2	1.66	0.43
4:D:48:LEU:HD23	4:D:54:LEU:HB2	2.01	0.43
4:D:115:PRO:HB2	4:D:193:ASP:HB3	2.01	0.43
5:E:133:GLU:OE2	5:E:141:THR:OG1	2.27	0.42
4:D:130:VAL:HG11	5:E:143:VAL:HG21	2.00	0.42
5:E:93:ILE:HG21	5:E:93:ILE:HD13	1.43	0.42
5:E:27:GLU:O	5:E:28:ASN:HB2	2.20	0.41
5:E:30:ARG:HB2	5:E:94:SER:O	2.20	0.41
1:A:146:LYS:HB3	1:A:146:LYS:HE3	1.44	0.41
1:A:169:ARG:HA	1:A:172:LEU:HD12	2.03	0.41
5:E:202:ASP:HA	5:E:203:PRO:HD3	1.83	0.41
1:A:258:THR:HG22	1:A:273:ARG:HB3	2.03	0.41
4:D:190:ILE:H	4:D:190:ILE:HG12	1.69	0.41
5:E:21:LEU:HD22	5:E:108:THR:HG21	2.03	0.41
1:A:218:GLN:HA	1:A:223:ASP:HA	2.02	0.41
5:E:52:VAL:HG12	5:E:53:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:THR:HA	2:B:72:PRO:HD2	1.93	0.40
1:A:192:HIS:NE2	2:B:98:ASP:O	2.55	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	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	194/195 (100%)	173 (89%)	20 (10%)	1 (0%)	24	55
5	E	240/242 (99%)	231 (96%)	6 (2%)	3 (1%)	9	31
All	All	813/822 (99%)	771 (95%)	38 (5%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	191	PRO
5	E	28	ASN
5	E	3	GLY
5	E	39	PRO

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	231/231 (100%)	208 (90%)	23 (10%)	7	24
2	B	96/95 (101%)	84 (88%)	12 (12%)	4	15
3	C	7/7 (100%)	5 (71%)	2 (29%)	0	1
4	D	173/172 (101%)	140 (81%)	33 (19%)	1	5
5	E	212/212 (100%)	183 (86%)	29 (14%)	3	13
All	All	719/717 (100%)	620 (86%)	99 (14%)	3	12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	95	VAL
1	A	110	LEU
1	A	121	LYS
1	A	128	GLU
1	A	146	LYS
1	A	163	THR
1	A	176	LYS
1	A	178	THR
1	A	194	VAL
1	A	196	ASP
1	A	197	HIS
1	A	214	THR
1	A	215	LEU
1	A	216	THR
1	A	223	ASP
1	A	225	THR
1	A	247	VAL
1	A	256	ARG
1	A	264	GLU
1	A	272	LEU
1	A	273	ARG
1	A	274	TRP
2	B	1	ILE
2	B	4	THR
2	B	6	LYS
2	B	9	VAL
2	B	16	GLU
2	B	21	ASN

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Mol	Chain	Res	Type
2	B	38	ASP
2	B	47	GLU
2	B	48	LYS
2	B	69	GLU
2	B	75	LYS
2	B	98	ASP
3	C	1	GLU
3	C	9	THR
4	D	2	GLN
4	D	12	ILE
4	D	18	VAL
4	D	20	MET
4	D	23	THR
4	D	25	SER
4	D	26	SER
4	D	27	ILE
4	D	30	THR
4	D	35	LYS
4	D	54	LEU
4	D	55	THR
4	D	60	LEU
4	D	63	GLN
4	D	64	PHE
4	D	66	ILE
4	D	73	LEU
4	D	79	ILE
4	D	95	GLN
4	D	100	THR
4	D	102	THR
4	D	104	LEU
4	D	105	THR
4	D	124	LYS
4	D	127	ASP
4	D	128	LYS
4	D	144	GLN
4	D	157	VAL
4	D	161	ARG
4	D	162	SER
4	D	169	SER
4	D	189	ILE
4	D	193	ASP
5	E	9	ARG

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Mol	Chain	Res	Type
5	E	17	THR
5	E	25	GLN
5	E	26	THR
5	E	27	GLU
5	E	29	HIS
5	E	39	PRO
5	E	46	ILE
5	E	60	VAL
5	E	66	VAL
5	E	69	SER
5	E	71	THR
5	E	77	THR
5	E	79	GLU
5	E	87	SER
5	E	93	ILE
5	E	94	SER
5	E	95	GLU
5	E	126	VAL
5	E	131	GLU
5	E	156	LEU
5	E	160	VAL
5	E	169	VAL
5	E	176	LEU
5	E	179	GLN
5	E	221	GLU
5	E	223	THR
5	E	225	ASP
5	E	243	ASP

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	54	GLN
1	A	141	GLN
1	A	191	HIS
2	B	13	HIS
2	B	89	GLN
4	D	2	GLN
4	D	21	ASN
4	D	175	ASN
4	D	187	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 [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	275/275 (100%)	-0.26	2 (0%) 84 77	18, 43, 82, 111	0
2	B	100/100 (100%)	-0.34	1 (1%) 79 72	27, 43, 78, 90	1 (1%)
3	C	10/10 (100%)	-0.41	0 100 100	29, 32, 37, 44	0
4	D	195/195 (100%)	0.30	8 (4%) 41 33	30, 56, 106, 119	1 (0%)
5	E	242/242 (100%)	-0.19	2 (0%) 82 75	26, 45, 73, 87	0
All	All	822/822 (100%)	-0.12	13 (1%) 70 61	18, 46, 86, 119	2 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	2	ALA	3.3
4	D	194	THR	3.2
4	D	189	ILE	2.9
4	D	55	THR	2.7
1	A	275	GLU	2.7
2	B	99[A]	MET	2.6
4	D	192	GLU	2.5
4	D	57	ASN	2.3
1	A	88	SER	2.3
4	D	51	ALA	2.3
4	D	195	PHE	2.2
4	D	196	PHE	2.0
5	E	183	ASN	2.0

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

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.