



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:10 AM BST

PDB ID : 6VRM
Title : T cell receptor-p53-HLA-A2 complex
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Deposited on : 2020-02-08
Resolution : 2.61 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	:	2.13.1
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)	:	2.13.1

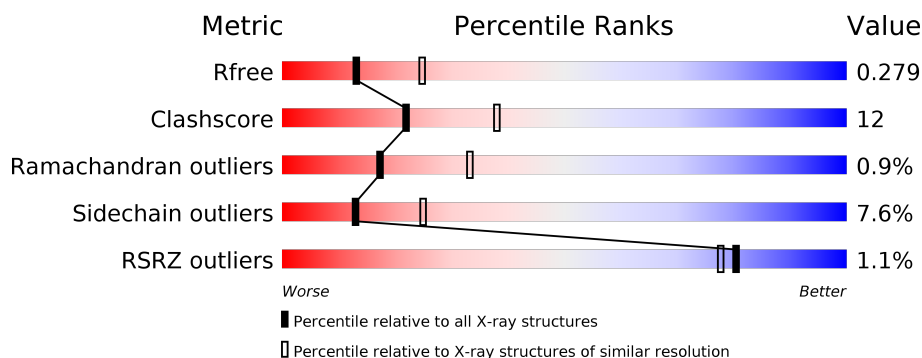
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	293	<div> <div>69%</div> <div>22%</div> <div>7%</div> </div>
2	B	100	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
3	D	205	<div> <div>3%</div> <div>73%</div> <div>15%</div> <div>11%</div> </div>
4	E	246	<div> <div>%</div> <div>66%</div> <div>28%</div> <div>5%</div> <div>.</div> </div>
5	P	9	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6303 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
			2172	1364	391	408	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q861F7
A	276	GLY	-	expression tag	UNP Q861F7
A	277	GLY	-	expression tag	UNP Q861F7
A	278	GLY	-	expression tag	UNP Q861F7
A	279	LEU	-	expression tag	UNP Q861F7
A	280	ASN	-	expression tag	UNP Q861F7
A	281	ASP	-	expression tag	UNP Q861F7
A	282	ILE	-	expression tag	UNP Q861F7
A	283	PHE	-	expression tag	UNP Q861F7
A	284	GLU	-	expression tag	UNP Q861F7
A	285	ALA	-	expression tag	UNP Q861F7
A	286	GLN	-	expression tag	UNP Q861F7
A	287	LYS	-	expression tag	UNP Q861F7
A	288	ILE	-	expression tag	UNP Q861F7
A	289	GLU	-	expression tag	UNP Q861F7
A	290	TRP	-	expression tag	UNP Q861F7
A	291	HIS	-	expression tag	UNP Q861F7
A	292	GLU	-	expression tag	UNP Q861F7

- 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
			781	498	131	149	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called T-cell receptor 12-6, alfa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	183	Total	C	N	O	S	0	0	0
			1388	874	224	282	8			

- Molecule 4 is a protein called TCR 12-6, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	244	Total	C	N	O	S	0	0	0
			1865	1173	320	363	9			

- Molecule 5 is a protein called Cellular tumor antigen p53 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			76	45	16	13	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	8	HIS	ARG	engineered mutation	UNP P04637

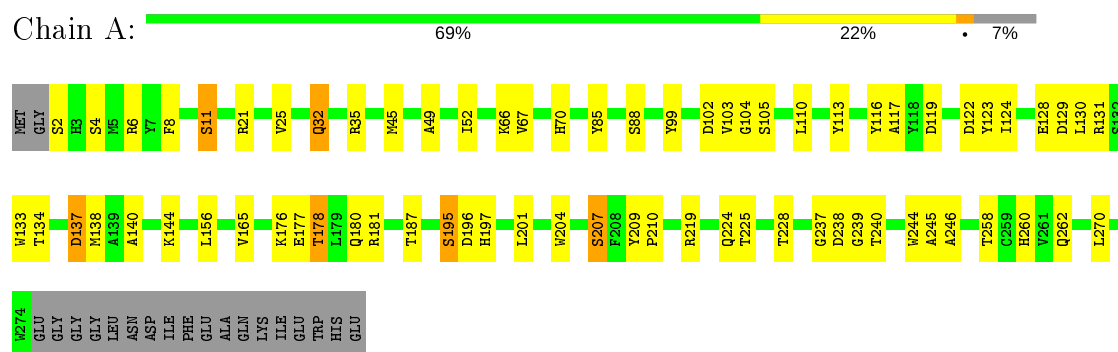
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	2	Total	O	0	0
			2	2		
6	D	3	Total	O	0	0
			3	3		
6	E	7	Total	O	0	0
			7	7		
6	P	2	Total	O	0	0
			2	2		

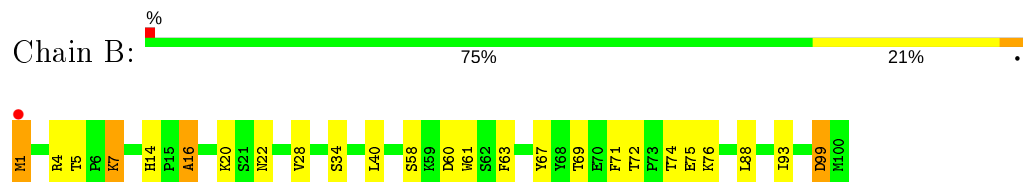
3 Residue-property plots [i](#)

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.

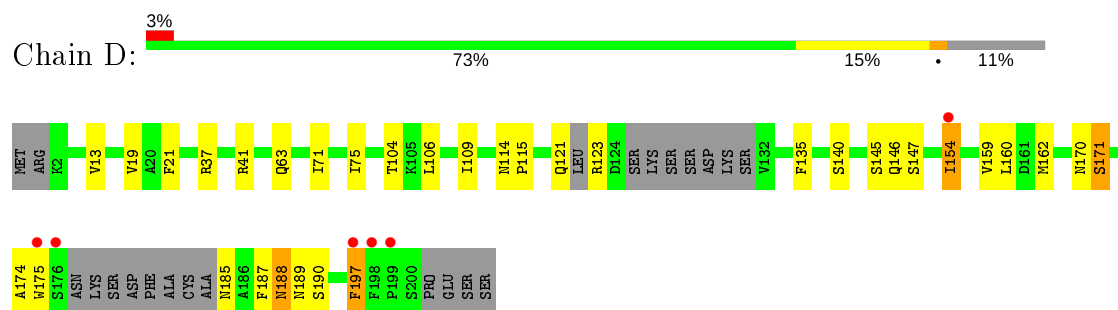
- Molecule 1: MHC class I antigen



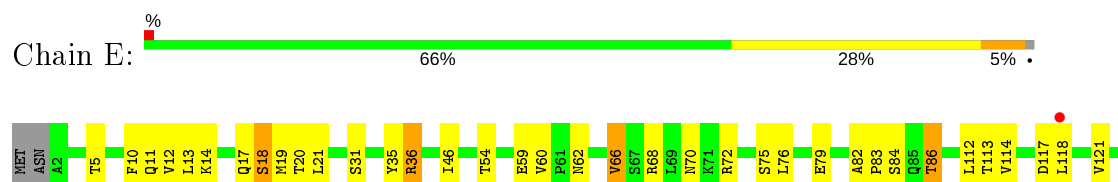
- Molecule 2: Beta-2-microglobulin

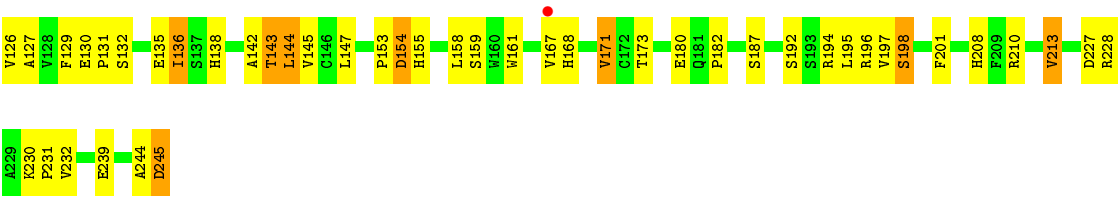


- Molecule 3: T-cell receptor 12-6, alfa chain

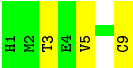


- Molecule 4: TCR 12-6, beta chain





• Molecule 5: Cellular tumor antigen p53 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.41Å 120.61Å 119.69Å 90.00° 108.38° 90.00°	Depositor
Resolution (Å)	19.79 – 2.61 37.86 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.79-2.61) 98.4 (37.86-2.61)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.275 0.195 , 0.279	Depositor DCC
R_{free} test set	1894 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6303	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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	0.58	0/2237	0.94	2/3048 (0.1%)
2	B	0.52	0/804	0.93	2/1100 (0.2%)
3	D	0.55	0/1418	0.91	1/1932 (0.1%)
4	E	0.64	1/1917 (0.1%)	0.95	4/2624 (0.2%)
5	P	0.74	0/77	1.00	0/101
All	All	0.59	1/6453 (0.0%)	0.94	9/8805 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	36	ARG	NE-CZ	14.18	1.51	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	36	ARG	NE-CZ-NH2	-13.46	113.57	120.30
4	E	36	ARG	NE-CZ-NH1	10.27	125.44	120.30
2	B	16	ALA	CB-CA-C	-6.88	99.78	110.10
3	D	37	ARG	CG-CD-NE	-5.75	99.72	111.80
4	E	68	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	32	GLN	CB-CA-C	5.29	120.99	110.40
2	B	4	ARG	CB-CG-CD	5.17	125.03	111.60
1	A	196	ASP	CB-CA-C	5.05	120.50	110.40
4	E	35	TYR	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2172	0	1980	46	0
2	B	781	0	690	17	0
3	D	1388	0	1253	32	0
4	E	1865	0	1685	60	0
5	P	76	0	74	2	0
6	A	7	0	0	0	0
6	B	2	0	0	0	0
6	D	3	0	0	0	0
6	E	7	0	0	1	0
6	P	2	0	0	0	0
All	All	6303	0	5682	141	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 12.

All (141) 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:E:143:THR:HG22	4:E:196:ARG:CG	1.73	1.15
4:E:143:THR:CG2	4:E:196:ARG:HG3	1.87	1.02
1:A:129:ASP:O	1:A:131:ARG:HG3	1.64	0.97
4:E:143:THR:HG22	4:E:196:ARG:HG3	0.96	0.96
4:E:167:VAL:HA	6:E:304:HOH:O	1.66	0.94
4:E:144:LEU:HD12	4:E:144:LEU:H	1.35	0.91
3:D:123:ARG:CB	4:E:130:GLU:HG2	2.04	0.87
3:D:185:ASN:HD21	3:D:188:ASN:HD21	1.20	0.87
1:A:6:ARG:NH1	1:A:113:TYR:OH	2.09	0.85
3:D:162:MET:CE	4:E:196:ARG:HD3	2.13	0.79
4:E:121:VAL:HG12	4:E:231:PRO:HB2	1.65	0.77
3:D:175:TRP:CD2	4:E:147:LEU:HD21	2.20	0.76
3:D:197:PHE:CD2	4:E:138:HIS:CD2	2.75	0.75
3:D:147:SER:N	3:D:154:ILE:HD11	2.01	0.75
2:B:74:THR:C	2:B:76:LYS:H	1.91	0.73
3:D:197:PHE:HD2	4:E:138:HIS:CD2	2.07	0.72
1:A:103:VAL:HA	1:A:110:LEU:HD13	1.70	0.72
4:E:144:LEU:HD12	4:E:144:LEU:N	2.07	0.70
4:E:18:SER:HB2	4:E:79:GLU:O	1.93	0.69
1:A:45:MET:HE2	1:A:67:VAL:HG11	1.74	0.67
3:D:162:MET:HE1	4:E:196:ARG:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HB2	1:A:224:GLN:OE1	1.96	0.66
3:D:41:ARG:NH2	4:E:154:ASP:OD2	2.29	0.66
4:E:59:GLU:HG2	4:E:60:VAL:HG13	1.78	0.66
2:B:60:ASP:O	2:B:61:TRP:HB2	1.96	0.65
3:D:185:ASN:HD21	3:D:188:ASN:ND2	1.92	0.65
2:B:74:THR:O	2:B:76:LYS:N	2.27	0.65
4:E:244:ALA:O	4:E:245:ASP:O	2.16	0.64
4:E:161:TRP:HB2	4:E:210:ARG:HB3	1.78	0.64
3:D:162:MET:HE2	4:E:196:ARG:HD3	1.81	0.62
1:A:4:SER:HB3	1:A:102:ASP:OD1	2.00	0.61
1:A:137:ASP:OD1	1:A:138:MET:N	2.34	0.60
4:E:14:LYS:H	4:E:17:GLN:HE21	1.49	0.60
3:D:171:SER:HB2	4:E:194:ARG:HE	1.67	0.59
3:D:159:VAL:HG22	3:D:170:ASN:OD1	2.03	0.59
1:A:207:SER:OG	1:A:207:SER:O	2.16	0.58
4:E:230:LYS:O	4:E:232:VAL:N	2.36	0.58
2:B:20:LYS:C	2:B:72:THR:HG22	2.25	0.57
4:E:144:LEU:CD1	4:E:144:LEU:H	2.12	0.57
4:E:11:GLN:HG2	4:E:19:MET:HE2	1.85	0.57
1:A:116:TYR:HB3	1:A:124:ILE:HG22	1.88	0.56
4:E:230:LYS:O	4:E:232:VAL:HG13	2.05	0.56
1:A:119:ASP:HB3	2:B:1:MET:HB3	1.89	0.55
1:A:201:LEU:O	1:A:246:ALA:HA	2.06	0.55
2:B:20:LYS:O	2:B:72:THR:HG22	2.07	0.55
1:A:49:ALA:O	1:A:52:ILE:HG22	2.07	0.54
2:B:99:ASP:OD1	2:B:99:ASP:N	2.39	0.54
4:E:143:THR:HA	4:E:195:LEU:O	2.07	0.54
1:A:207:SER:HA	1:A:240:THR:HB	1.89	0.54
3:D:21:PHE:HE1	3:D:104:THR:HG22	1.72	0.54
4:E:126:VAL:HG21	4:E:213:VAL:CG1	2.38	0.54
3:D:121:GLN:O	4:E:132:SER:HB2	2.08	0.54
3:D:21:PHE:HZ	3:D:106:LEU:HB2	1.73	0.53
3:D:21:PHE:CE1	3:D:104:THR:CG2	2.92	0.53
1:A:45:MET:CE	1:A:67:VAL:HB	2.39	0.52
2:B:74:THR:C	2:B:76:LYS:N	2.60	0.52
1:A:45:MET:HE1	1:A:67:VAL:HB	1.92	0.52
4:E:168:HIS:O	4:E:171:VAL:HG13	2.09	0.52
4:E:135:GLU:OE2	4:E:143:THR:HG23	2.10	0.52
4:E:11:GLN:HG2	4:E:19:MET:CE	2.39	0.51
4:E:10:PHE:CD2	4:E:155:HIS:HB3	2.45	0.51
4:E:180:GLU:O	4:E:182:PRO:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:86:THR:HB	4:E:113:THR:HA	1.92	0.51
1:A:8:PHE:CD1	1:A:8:PHE:N	2.78	0.51
4:E:143:THR:HG22	4:E:196:ARG:CD	2.39	0.51
2:B:93:ILE:O	2:B:93:ILE:HD12	2.11	0.51
3:D:21:PHE:HE1	3:D:104:THR:CG2	2.23	0.50
3:D:154:ILE:HG22	3:D:174:ALA:HB2	1.93	0.50
4:E:10:PHE:HB3	4:E:155:HIS:ND1	2.26	0.50
4:E:18:SER:CB	4:E:79:GLU:O	2.59	0.50
1:A:187:THR:HA	1:A:204:TRP:O	2.12	0.50
2:B:34:SER:HB3	2:B:63:PHE:CE2	2.47	0.50
1:A:195:SER:HB3	1:A:197:HIS:H	1.77	0.49
1:A:237:GLY:C	1:A:239:GLY:H	2.16	0.49
4:E:143:THR:CG2	4:E:196:ARG:CG	2.66	0.49
3:D:123:ARG:CB	4:E:130:GLU:CG	2.87	0.49
4:E:136:ILE:HG23	4:E:142:ALA:HB2	1.95	0.49
1:A:128:GLU:O	1:A:130:LEU:HD13	2.13	0.49
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.48	0.48
1:A:133:TRP:HB2	1:A:144:LYS:HD2	1.95	0.48
5:P:3:THR:OG1	5:P:5:VAL:HG23	2.14	0.48
3:D:21:PHE:CD1	3:D:104:THR:HG21	2.48	0.48
2:B:5:THR:HG23	2:B:88:LEU:HD21	1.96	0.47
1:A:130:LEU:CD1	1:A:130:LEU:N	2.77	0.47
1:A:130:LEU:HD12	1:A:130:LEU:N	2.29	0.47
4:E:13:LEU:O	4:E:114:VAL:HA	2.14	0.47
4:E:86:THR:HA	4:E:112:LEU:O	2.14	0.47
4:E:21:LEU:N	4:E:21:LEU:HD12	2.30	0.47
3:D:145:SER:N	3:D:190:SER:OG	2.39	0.47
4:E:70:ASN:OD1	4:E:72:ARG:HB3	2.14	0.46
1:A:225:THR:HA	1:A:228:THR:OG1	2.16	0.46
1:A:103:VAL:CA	1:A:110:LEU:HD13	2.41	0.46
3:D:21:PHE:CE1	3:D:104:THR:HG21	2.51	0.46
1:A:244:TRP:HE3	1:A:245:ALA:N	2.14	0.46
4:E:36:ARG:HB3	4:E:46:ILE:HD11	1.98	0.46
4:E:82:ALA:HB1	4:E:83:PRO:HD2	1.98	0.45
4:E:153:PRO:O	4:E:155:HIS:N	2.43	0.45
3:D:197:PHE:CE2	4:E:138:HIS:CD2	3.05	0.45
2:B:40:LEU:HD12	2:B:69:THR:HG22	1.98	0.45
1:A:130:LEU:H	1:A:130:LEU:HD12	1.81	0.45
4:E:66:VAL:HA	4:E:75:SER:O	2.17	0.45
1:A:258:THR:OG1	1:A:260:HIS:NE2	2.38	0.45
3:D:197:PHE:HD2	4:E:138:HIS:NE2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:VAL:HG12	3:D:75:ILE:HB	1.98	0.45
4:E:158:LEU:HD23	4:E:159:SER:N	2.32	0.44
1:A:134:THR:O	1:A:134:THR:OG1	2.30	0.44
4:E:198:SER:HB2	4:E:201:PHE:CB	2.47	0.44
5:P:3:THR:HG23	5:P:5:VAL:H	1.82	0.44
1:A:102:ASP:OD2	1:A:113:TYR:HE2	2.01	0.44
3:D:123:ARG:CB	4:E:130:GLU:O	2.66	0.44
2:B:14:HIS:O	2:B:22:ASN:ND2	2.46	0.43
4:E:208:HIS:HE1	4:E:239:GLU:OE2	2.01	0.43
3:D:135:PHE:HB2	3:D:187:PHE:CE2	2.54	0.43
4:E:117:ASP:OD1	4:E:118:LEU:N	2.53	0.42
1:A:66:LYS:O	1:A:70:HIS:HD2	2.02	0.42
2:B:7:LYS:O	2:B:28:VAL:HA	2.19	0.42
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.23	0.42
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.54	0.42
1:A:70:HIS:HE1	1:A:99:TYR:OH	2.02	0.42
1:A:25:VAL:HG23	1:A:32:GLN:OE1	2.19	0.42
1:A:104:GLY:N	1:A:110:LEU:HD11	2.35	0.42
1:A:176:LYS:HA	1:A:180:GLN:HG3	2.02	0.42
4:E:131:PRO:HD3	4:E:144:LEU:HG	2.02	0.42
1:A:209:TYR:HA	1:A:210:PRO:O	2.20	0.41
1:A:45:MET:CE	1:A:67:VAL:CB	2.98	0.41
4:E:83:PRO:O	4:E:86:THR:HG23	2.21	0.41
4:E:70:ASN:C	4:E:72:ARG:H	2.24	0.41
2:B:93:ILE:HG13	2:B:93:ILE:H	1.66	0.41
4:E:127:ALA:HB3	4:E:129:PHE:HE1	1.85	0.41
3:D:146:GLN:O	3:D:189:ASN:ND2	2.51	0.41
1:A:104:GLY:N	1:A:110:LEU:CD1	2.84	0.41
4:E:59:GLU:O	4:E:59:GLU:HG2	2.20	0.41
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.90	0.41
1:A:176:LYS:O	1:A:178:THR:N	2.54	0.41
1:A:70:HIS:CE1	1:A:99:TYR:OH	2.74	0.41
1:A:11:SER:HA	1:A:21:ARG:O	2.21	0.40
1:A:237:GLY:C	1:A:239:GLY:N	2.75	0.40
3:D:109:ILE:CG2	3:D:140:SER:HB3	2.51	0.40
3:D:114:ASN:O	3:D:115:PRO:C	2.59	0.40
2:B:67:TYR:CD1	2:B:67:TYR:N	2.89	0.40
3:D:63:GLN:O	3:D:71:ILE:HA	2.21	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	271/293 (92%)	245 (90%)	24 (9%)	2 (1%)	22	41
2	B	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	7	13
3	D	175/205 (85%)	167 (95%)	8 (5%)	0	100	100
4	E	242/246 (98%)	211 (87%)	28 (12%)	3 (1%)	13	25
5	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	793/853 (93%)	719 (91%)	67 (8%)	7 (1%)	17	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	177	GLU
2	B	16	ALA
4	E	154	ASP
2	B	75	GLU
4	E	62	ASN
4	E	198	SER

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	215/245 (88%)	201 (94%)	14 (6%)	17	33
2	B	81/95 (85%)	76 (94%)	5 (6%)	18	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	151/185 (82%)	145 (96%)	6 (4%)	31	55
4	E	192/213 (90%)	169 (88%)	23 (12%)	5	8
5	P	9/9 (100%)	8 (89%)	1 (11%)	6	10
All	All	648/747 (87%)	599 (92%)	49 (8%)	13	25

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	11	SER
1	A	35	ARG
1	A	88	SER
1	A	105	SER
1	A	137	ASP
1	A	165	VAL
1	A	178	THR
1	A	181	ARG
1	A	195	SER
1	A	207	SER
1	A	238	ASP
1	A	262	GLN
1	A	270	LEU
2	B	1	MET
2	B	7	LYS
2	B	58	SER
2	B	71	PHE
2	B	99	ASP
3	D	13	VAL
3	D	154	ILE
3	D	160	LEU
3	D	171	SER
3	D	188	ASN
3	D	197	PHE
4	E	5	THR
4	E	12	VAL
4	E	18	SER
4	E	20	THR
4	E	31	SER
4	E	54	THR
4	E	66	VAL
4	E	76	LEU

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Mol	Chain	Res	Type
4	E	84	SER
4	E	86	THR
4	E	136	ILE
4	E	143	THR
4	E	144	LEU
4	E	145	VAL
4	E	171	VAL
4	E	173	THR
4	E	187	SER
4	E	192	SER
4	E	197	VAL
4	E	213	VAL
4	E	227	ASP
4	E	228	ARG
4	E	245	ASP
5	P	9	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	86	ASN
1	A	180	GLN
3	D	185	ASN
4	E	17	GLN
4	E	138	HIS
4	E	208	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	273/293 (93%)	-0.39	0 100 100	52, 75, 95, 112	0
2	B	100/100 (100%)	-0.29	1 (1%) 82 80	56, 82, 108, 116	0
3	D	183/205 (89%)	-0.09	6 (3%) 46 40	53, 68, 107, 127	0
4	E	244/246 (99%)	-0.29	2 (0%) 86 84	54, 85, 109, 122	0
5	P	9/9 (100%)	0.37	0 100 100	56, 59, 69, 76	0
All	All	809/853 (94%)	-0.27	9 (1%) 80 78	52, 77, 106, 127	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	197	PHE	3.0
3	D	175	TRP	2.8
3	D	154	ILE	2.6
2	B	1	MET	2.5
4	E	167	VAL	2.4
3	D	176	SER	2.4
3	D	199	PRO	2.3
4	E	118	LEU	2.0
3	D	198	PHE	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.