Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:20 AM JST

PDB ID	:	7F4W
Title	:	Complex structure of HLA2402 with recognizing SARS-CoV-2 epitope pep4
Authors	:	Deng, S.; Jin, T.
Deposited on	:	2021-06-21
Resolution	:	2.90 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:

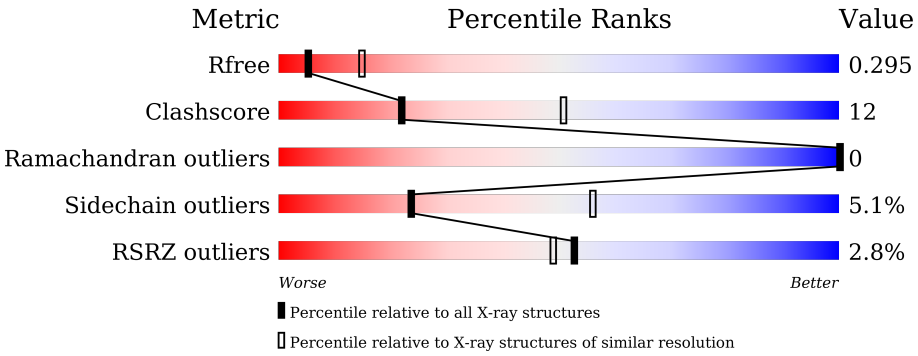
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	308	4% 63% 27% • 9%
1	C	308	3% 59% 29% • 9%
2	B	102	% 75% 23% •
2	D	102	% 72% 25% • •
3	E	9	78% 22%
3	F	9	56% 33% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6388 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	280	Total	C	N	O	S	0	0	0
			2267	1408	410	438	11			
1	C	280	Total	C	N	O	S	0	0	0
			2267	1408	410	438	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP D9UAY1
A	-3	ASN	-	expression tag	UNP D9UAY1
A	-2	SER	-	expression tag	UNP D9UAY1
A	-1	VAL	-	expression tag	UNP D9UAY1
A	0	ASP	-	expression tag	UNP D9UAY1
A	277	GLY	-	expression tag	UNP D9UAY1
A	278	SER	-	expression tag	UNP D9UAY1
A	279	GLY	-	expression tag	UNP D9UAY1
A	280	LEU	-	expression tag	UNP D9UAY1
A	281	ASN	-	expression tag	UNP D9UAY1
A	282	ASP	-	expression tag	UNP D9UAY1
A	283	ILE	-	expression tag	UNP D9UAY1
A	284	PHE	-	expression tag	UNP D9UAY1
A	285	GLU	-	expression tag	UNP D9UAY1
A	286	ALA	-	expression tag	UNP D9UAY1
A	287	GLN	-	expression tag	UNP D9UAY1
A	288	LYS	-	expression tag	UNP D9UAY1
A	289	ILE	-	expression tag	UNP D9UAY1
A	290	GLU	-	expression tag	UNP D9UAY1
A	291	TRP	-	expression tag	UNP D9UAY1
A	292	HIS	-	expression tag	UNP D9UAY1
A	293	ALA	-	expression tag	UNP D9UAY1
A	294	ALA	-	expression tag	UNP D9UAY1
A	295	ALA	-	expression tag	UNP D9UAY1
A	296	LEU	-	expression tag	UNP D9UAY1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLU	-	expression tag	UNP D9UAY1
A	298	HIS	-	expression tag	UNP D9UAY1
A	299	HIS	-	expression tag	UNP D9UAY1
A	300	HIS	-	expression tag	UNP D9UAY1
A	301	HIS	-	expression tag	UNP D9UAY1
A	302	HIS	-	expression tag	UNP D9UAY1
A	303	HIS	-	expression tag	UNP D9UAY1
C	-4	MET	-	initiating methionine	UNP D9UAY1
C	-3	ASN	-	expression tag	UNP D9UAY1
C	-2	SER	-	expression tag	UNP D9UAY1
C	-1	VAL	-	expression tag	UNP D9UAY1
C	0	ASP	-	expression tag	UNP D9UAY1
C	277	GLY	-	expression tag	UNP D9UAY1
C	278	SER	-	expression tag	UNP D9UAY1
C	279	GLY	-	expression tag	UNP D9UAY1
C	280	LEU	-	expression tag	UNP D9UAY1
C	281	ASN	-	expression tag	UNP D9UAY1
C	282	ASP	-	expression tag	UNP D9UAY1
C	283	ILE	-	expression tag	UNP D9UAY1
C	284	PHE	-	expression tag	UNP D9UAY1
C	285	GLU	-	expression tag	UNP D9UAY1
C	286	ALA	-	expression tag	UNP D9UAY1
C	287	GLN	-	expression tag	UNP D9UAY1
C	288	LYS	-	expression tag	UNP D9UAY1
C	289	ILE	-	expression tag	UNP D9UAY1
C	290	GLU	-	expression tag	UNP D9UAY1
C	291	TRP	-	expression tag	UNP D9UAY1
C	292	HIS	-	expression tag	UNP D9UAY1
C	293	ALA	-	expression tag	UNP D9UAY1
C	294	ALA	-	expression tag	UNP D9UAY1
C	295	ALA	-	expression tag	UNP D9UAY1
C	296	LEU	-	expression tag	UNP D9UAY1
C	297	GLU	-	expression tag	UNP D9UAY1
C	298	HIS	-	expression tag	UNP D9UAY1
C	299	HIS	-	expression tag	UNP D9UAY1
C	300	HIS	-	expression tag	UNP D9UAY1
C	301	HIS	-	expression tag	UNP D9UAY1
C	302	HIS	-	expression tag	UNP D9UAY1
C	303	HIS	-	expression tag	UNP D9UAY1

- 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
			837	533	141	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	VAL	-	expression tag	UNP P61769
B	-1	ASP	-	expression tag	UNP P61769
B	0	MET	-	expression tag	UNP P61769
D	-2	VAL	-	expression tag	UNP P61769
D	-1	ASP	-	expression tag	UNP P61769
D	0	MET	-	expression tag	UNP P61769

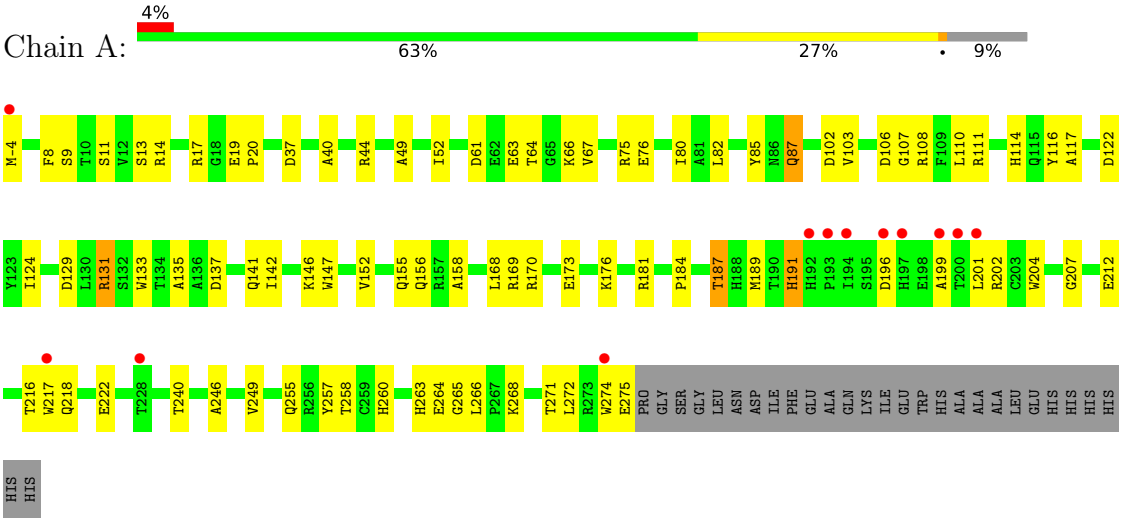
- Molecule 3 is a protein called SARS-CoV-2 T-cell Epitope pep4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			90	62	14	14			
3	F	9	Total	C	N	O	0	0	0
			90	62	14	14			

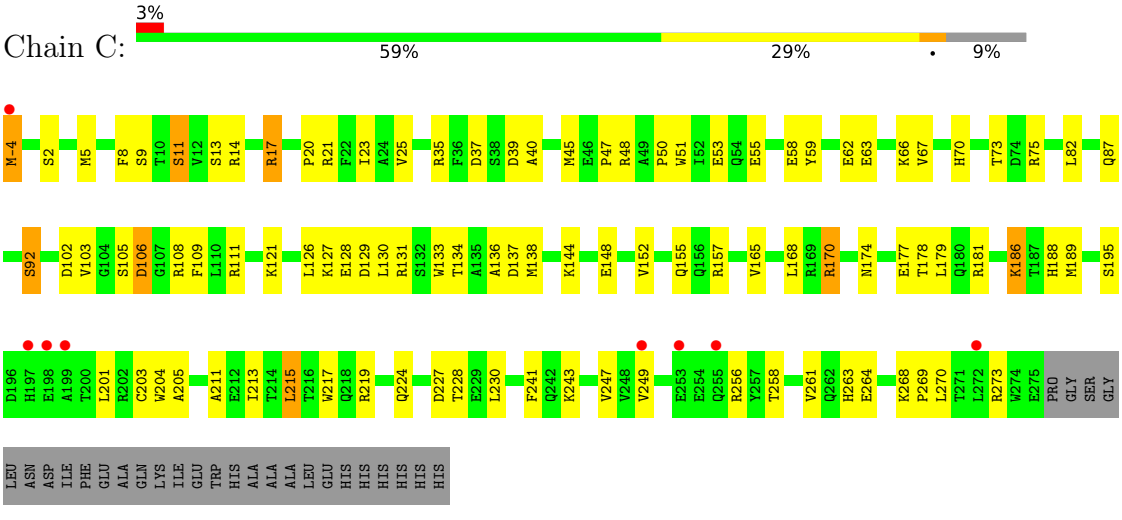
3 Residue-property plots (i)

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.

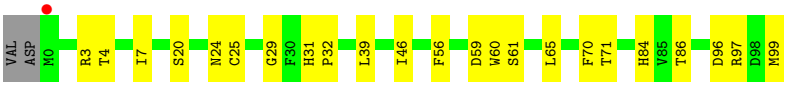
• Molecule 1: MHC class I antigen



• Molecule 1: MHC class I antigen

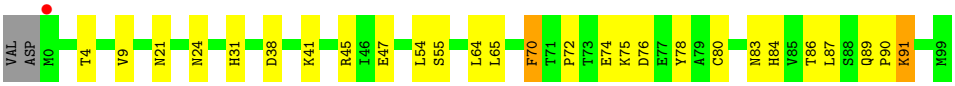


• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin

Chain D:

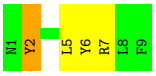


• Molecule 3: SARS-CoV-2 T-cell Epitope pep4

Chain E:

• Molecule 3: SARS-CoV-2 T-cell Epitope pep4

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.44Å 135.60Å 153.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 2.90 47.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.83-2.90) 90.2 (47.83-2.90)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.244 , 0.298 0.241 , 0.295	Depositor DCC
R_{free} test set	1132 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.49	0/2327	0.68	0/3154
1	C	0.49	0/2327	0.71	1/3154 (0.0%)
2	B	0.55	0/860	0.64	0/1162
2	D	0.51	0/860	0.69	0/1162
3	E	0.51	0/93	0.69	0/125
3	F	0.52	0/93	0.75	0/125
All	All	0.50	0/6560	0.69	1/8882 (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
1	C	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	-4	MET	CG-SD-CE	-10.91	82.74	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	106	ASP	Peptide
1	C	195	SER	Peptide

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	2267	0	2121	60	0
1	C	2267	0	2121	61	1
2	B	837	0	803	11	0
2	D	837	0	803	17	0
3	E	90	0	85	4	0
3	F	90	0	85	5	0
All	All	6388	0	6018	146	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 12.

All (146) 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:C:261:VAL:HG22	1:C:270:LEU:HB2	1.53	0.89
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.60	0.82
1:C:106:ASP:HB2	1:C:108:ARG:H	1.47	0.80
1:C:102:ASP:HB2	1:C:111:ARG:HG3	1.67	0.76
1:A:-4:MET:HG3	1:A:264:GLU:OE1	1.85	0.76
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.69	0.75
1:A:187:THR:HB	1:A:272:LEU:HD21	1.69	0.74
1:C:55:GLU:OE1	1:C:170:ARG:NH2	2.20	0.74
1:A:20:PRO:HG2	1:A:75:ARG:HG2	1.71	0.73
1:A:44:ARG:HD2	1:A:64:THR:HG21	1.70	0.73
3:F:7:ARG:HG3	3:F:7:ARG:HH11	1.53	0.72
1:A:255:GLN:HE22	1:A:275:GLU:H	1.39	0.71
1:C:219:ARG:HD3	1:C:256:ARG:NH1	2.07	0.70
1:A:156:GLN:HE22	3:E:3:ASN:HD21	1.42	0.68
1:C:14:ARG:HB3	1:C:17:ARG:HB2	1.75	0.68
2:D:87:LEU:HD22	2:D:91:LYS:HD3	1.76	0.68
1:A:191:HIS:CE1	1:A:199:ALA:HB1	2.30	0.67
2:D:45:ARG:NH2	2:D:47:GLU:OE1	2.29	0.66
2:D:9:VAL:HG21	2:D:80:CYS:HB2	1.78	0.65
1:A:102:ASP:HB2	1:A:111:ARG:HB2	1.78	0.64
2:D:74:GLU:OE1	2:D:74:GLU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASP:OD2	1:A:131:ARG:HB2	1.97	0.63
1:A:103:VAL:HG23	1:A:168:LEU:HD23	1.80	0.63
1:C:63:GLU:O	1:C:67:VAL:HG23	1.99	0.63
1:A:173:GLU:O	1:A:176:LYS:HG3	2.00	0.60
1:A:170:ARG:NH2	3:E:1:ASN:OD1	2.35	0.59
2:D:70:PHE:CZ	2:D:72:PRO:HG3	2.36	0.59
1:C:144:LYS:NZ	1:C:148:GLU:OE2	2.35	0.59
1:C:13:SER:O	1:C:92:SER:HB2	2.03	0.59
1:C:8:PHE:HB2	1:C:25:VAL:HG23	1.85	0.58
1:C:51:TRP:CZ2	1:C:179:LEU:HD11	2.39	0.58
2:D:4:THR:HG22	2:D:86:THR:HB	1.83	0.58
1:C:109:PHE:HB2	1:C:165:VAL:HG21	1.86	0.58
1:A:142:ILE:O	1:A:146:LYS:HG3	2.04	0.57
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.11	0.57
1:A:249:VAL:HG23	1:A:257:TYR:CZ	2.39	0.56
1:C:189:MET:HE1	1:C:273:ARG:C	2.27	0.55
1:C:20:PRO:HD2	1:C:75:ARG:HG2	1.89	0.55
1:C:35:ARG:HD3	1:C:48:ARG:HD2	1.88	0.55
1:C:268:LYS:HD2	1:C:269:PRO:HD2	1.89	0.55
1:A:218:GLN:HA	1:A:222:GLU:O	2.07	0.54
1:C:178:THR:O	1:C:181:ARG:HB3	2.07	0.54
1:C:11:SER:HA	1:C:21:ARG:O	2.07	0.54
1:C:205:ALA:HB2	1:C:215:LEU:HD21	1.89	0.54
1:C:45:MET:CG	1:C:67:VAL:HG21	2.39	0.53
1:A:191:HIS:HE1	1:A:199:ALA:HB1	1.71	0.53
1:C:224:GLN:O	1:C:228:THR:HG23	2.09	0.53
1:A:133:TRP:HZ2	1:A:152:VAL:HG13	1.74	0.52
1:C:219:ARG:HD3	1:C:256:ARG:HH12	1.73	0.52
1:A:189:MET:HE1	1:A:217:TRP:HH2	1.75	0.51
1:C:25:VAL:HG21	2:D:55:SER:HB3	1.92	0.51
1:A:-4:MET:HG3	1:A:264:GLU:CD	2.32	0.50
1:C:177:GLU:O	1:C:181:ARG:HB2	2.12	0.50
1:A:147:TRP:HB3	1:A:152:VAL:HG11	1.93	0.50
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.46	0.49
1:A:106:ASP:HB3	1:A:108:ARG:HD3	1.93	0.49
1:C:227:ASP:O	1:C:247:VAL:HG23	2.12	0.49
1:A:63:GLU:O	1:A:67:VAL:HG12	2.12	0.49
1:C:126:LEU:HB2	1:C:133:TRP:CZ3	2.48	0.49
1:A:249:VAL:HG23	1:A:257:TYR:CE1	2.48	0.48
1:C:128:GLU:H	1:C:128:GLU:CD	2.16	0.48
2:B:20:SER:HA	2:B:71:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:PRO:O	1:C:48:ARG:HG2	2.13	0.48
1:C:5:MET:HB2	1:C:168:LEU:HD13	1.93	0.48
1:C:127:LYS:HE3	1:C:127:LYS:HB3	1.62	0.48
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.49	0.48
1:A:135:ALA:HB3	1:A:141:GLN:HG3	1.95	0.48
1:A:147:TRP:HB3	1:A:152:VAL:CG1	2.43	0.48
1:A:156:GLN:NE2	3:E:3:ASN:HD21	2.08	0.48
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.96	0.48
1:A:13:SER:HA	1:A:20:PRO:HB3	1.96	0.47
1:C:130:LEU:HB2	1:C:157:ARG:HD3	1.95	0.47
1:C:106:ASP:HB2	1:C:108:ARG:N	2.23	0.47
2:D:89:GLN:HB2	2:D:90:PRO:CD	2.44	0.47
1:A:201:LEU:HD21	1:A:274:TRP:CD1	2.50	0.47
1:A:212:GLU:O	1:A:263:HIS:CD2	2.68	0.46
1:C:23:ILE:HG21	2:D:54:LEU:HB3	1.97	0.46
1:C:-4:MET:HB3	1:C:264:GLU:OE2	2.16	0.46
1:C:45:MET:HG2	1:C:67:VAL:HG21	1.97	0.46
1:C:188:HIS:O	1:C:204:TRP:HB2	2.15	0.46
1:C:213:ILE:HG13	1:C:263:HIS:HB2	1.98	0.46
1:A:116:TYR:HB2	1:A:124:ILE:HG22	1.96	0.46
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.31	0.46
1:A:114:HIS:NE2	1:A:156:GLN:NE2	2.63	0.46
1:A:268:LYS:HD2	1:A:268:LYS:HA	1.47	0.46
1:C:55:GLU:CD	1:C:170:ARG:HH21	2.19	0.46
2:B:39:LEU:O	2:B:46:ILE:HG13	2.15	0.45
1:A:184:PRO:HB3	1:A:265:GLY:O	2.15	0.45
1:A:14:ARG:HB3	1:A:17:ARG:HB2	1.99	0.45
1:C:186:LYS:NZ	1:C:188:HIS:HB3	2.32	0.45
1:A:82:LEU:HD12	1:A:87:GLN:HG3	1.98	0.45
1:C:130:LEU:HD12	1:C:157:ARG:HG3	1.99	0.45
1:C:129:ASP:O	1:C:131:ARG:HG3	2.17	0.45
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.52	0.44
1:A:103:VAL:HG23	1:A:168:LEU:CD2	2.46	0.44
1:A:189:MET:HE2	1:A:189:MET:HB2	1.57	0.44
2:B:7:ILE:HD11	2:B:25:CYS:SG	2.58	0.44
1:C:217:TRP:HB2	1:C:228:THR:HG22	1.99	0.44
1:C:73:THR:OG1	3:F:6:TYR:HA	2.18	0.44
1:C:258:THR:HG22	1:C:273:ARG:HG2	1.99	0.44
1:A:49:ALA:O	1:A:52:ILE:HG22	2.17	0.44
2:B:96:ASP:HB3	2:B:99:MET:HA	2.00	0.44
1:C:37:ASP:HB3	1:C:40:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:HIS:CG	3:F:5:LEU:HD12	2.53	0.44
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.71	0.43
1:C:8:PHE:HB2	1:C:25:VAL:CG2	2.47	0.43
1:C:45:MET:CE	1:C:67:VAL:HG21	2.48	0.43
2:D:83:ASN:HB2	2:D:90:PRO:HG3	2.00	0.43
1:A:37:ASP:HB3	1:A:40:ALA:HB2	2.00	0.43
1:C:58:GLU:O	1:C:62:GLU:HG3	2.18	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.43
1:C:211:ALA:HB2	1:C:241:PHE:CE2	2.53	0.43
2:D:31:HIS:O	2:D:84:HIS:HE1	2.01	0.43
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.99	0.43
1:A:202:ARG:HG3	1:A:246:ALA:HB2	2.00	0.43
1:A:202:ARG:HD3	1:A:204:TRP:CZ2	2.54	0.43
1:A:207:GLY:HA2	1:A:240:THR:OG1	2.18	0.43
2:B:59:ASP:OD1	2:B:61:SER:OG	2.22	0.43
2:B:84:HIS:ND1	2:B:86:THR:HG23	2.34	0.42
1:C:66:LYS:HE3	3:F:2:TYR:HB3	2.00	0.42
1:C:230:LEU:HD11	1:C:243:LYS:HE3	2.00	0.42
1:A:155:GLN:O	1:A:158:ALA:HB3	2.20	0.42
1:C:21:ARG:HD2	1:C:39:ASP:OD2	2.19	0.42
1:A:44:ARG:HH12	1:A:61:ASP:HA	1.83	0.42
1:A:66:LYS:HD2	3:E:3:ASN:O	2.18	0.42
1:A:76:GLU:O	1:A:80:ILE:HG12	2.20	0.42
1:A:191:HIS:HB2	1:A:274:TRP:NE1	2.35	0.42
1:C:50:PRO:O	1:C:53:GLU:HG2	2.20	0.42
1:C:59:TYR:O	1:C:63:GLU:HG2	2.19	0.42
1:C:152:VAL:HG22	3:F:7:ARG:NH1	2.34	0.42
1:A:8:PHE:HD1	2:B:56:PHE:CE1	2.38	0.42
2:D:47:GLU:O	2:D:47:GLU:HG3	2.20	0.42
1:A:147:TRP:O	1:A:152:VAL:HG12	2.21	0.41
1:A:187:THR:HA	1:A:204:TRP:O	2.21	0.41
1:C:82:LEU:HD22	1:C:87:GLN:HB2	2.02	0.41
2:D:38:ASP:HB3	2:D:45:ARG:HG3	2.02	0.41
1:A:189:MET:HE1	1:A:217:TRP:CH2	2.54	0.41
1:A:189:MET:CE	1:A:201:LEU:HD22	2.51	0.41
1:C:201:LEU:HD21	1:C:217:TRP:CH2	2.56	0.41
2:D:41:LYS:HE3	2:D:78:TYR:OH	2.21	0.41
1:A:201:LEU:O	1:A:246:ALA:HA	2.21	0.40
1:A:107:GLY:O	1:A:169:ARG:HD2	2.21	0.40
1:C:258:THR:HG22	1:C:273:ARG:CG	2.51	0.40
2:D:75:LYS:HG3	2:D:76:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:C	1:A:268:LYS:H	2.25	0.40
1:C:121:LYS:NZ	1:C:136:ALA:HB1	2.37	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:17:ARG:NH2	1:C:174:ASN:OD1[1_455]	2.16	0.04

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	278/308 (90%)	266 (96%)	12 (4%)	0	100	100
1	C	278/308 (90%)	265 (95%)	13 (5%)	0	100	100
2	B	98/102 (96%)	96 (98%)	2 (2%)	0	100	100
2	D	98/102 (96%)	93 (95%)	5 (5%)	0	100	100
3	E	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	766/838 (91%)	733 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	236/258 (92%)	224 (95%)	12 (5%)	24 56
1	C	236/258 (92%)	221 (94%)	15 (6%)	17 45
2	B	95/97 (98%)	91 (96%)	4 (4%)	30 63
2	D	95/97 (98%)	92 (97%)	3 (3%)	39 73
3	E	9/9 (100%)	9 (100%)	0	100 100
3	F	9/9 (100%)	8 (89%)	1 (11%)	6 19
All	All	680/728 (93%)	645 (95%)	35 (5%)	24 56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	SER
1	A	87	GLN
1	A	110	LEU
1	A	122	ASP
1	A	131	ARG
1	A	181	ARG
1	A	187	THR
1	A	191	HIS
1	A	196	ASP
1	A	216	THR
1	A	258	THR
2	B	3	ARG
2	B	4	THR
2	B	70	PHE
2	B	97	ARG
1	C	2	SER
1	C	9	SER
1	C	11	SER
1	C	17	ARG
1	C	92	SER
1	C	103	VAL
1	C	105	SER
1	C	134	THR
1	C	137	ASP
1	C	138	MET
1	C	155	GLN
1	C	170	ARG

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Mol	Chain	Res	Type
1	C	186	LYS
1	C	215	LEU
1	C	249	VAL
2	D	64	LEU
2	D	70	PHE
2	D	91	LYS
3	F	2	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	255	GLN
1	C	226	GLN
2	D	24	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 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, 95^{th} 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	280/308 (90%)	0.42	12 (4%) 35 31	45, 62, 96, 111	0
1	C	280/308 (90%)	0.41	8 (2%) 51 47	46, 59, 99, 143	0
2	B	100/102 (98%)	0.26	1 (1%) 82 82	48, 56, 79, 102	0
2	D	100/102 (98%)	0.29	1 (1%) 82 82	47, 60, 85, 96	0
3	E	9/9 (100%)	0.68	0 100 100	53, 59, 64, 73	0
3	F	9/9 (100%)	0.33	0 100 100	52, 56, 60, 61	0
All	All	778/838 (92%)	0.38	22 (2%) 53 49	45, 60, 90, 143	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	ALA	6.7
1	C	197	HIS	5.8
1	A	197	HIS	3.8
1	A	200	THR	3.7
2	B	0	MET	3.7
2	D	0	MET	3.4
1	A	199	ALA	3.2
1	C	255	GLN	3.0
1	A	201	LEU	2.7
1	A	194	ILE	2.7
1	C	253	GLU	2.7
1	A	274	TRP	2.4
1	C	272	LEU	2.4
1	A	192	HIS	2.3
1	C	-4	MET	2.3
1	A	217	TRP	2.3
1	A	-4	MET	2.2
1	A	228	THR	2.2
1	C	249	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	196	ASP	2.1
1	A	193	PRO	2.0
1	C	198	GLU	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.