



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 AM GMT

PDB ID : 2ZSW  
Title : Crystal structure of H-2Kb in complex with the Q600Y variant of JHNV epitope S598  
Authors : Theodossis, A.; Dunstone, M.A.; Rossjohn, J.  
Deposited on : 2008-09-18  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

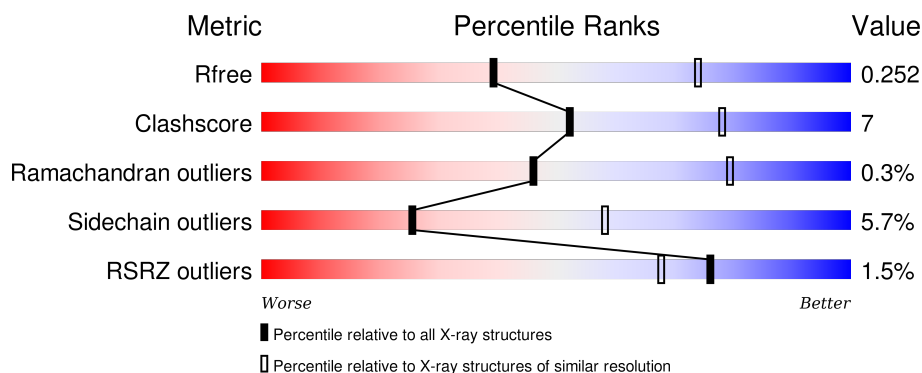
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	278	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	278	<div> <div>%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	278	<div> <div>%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	G	278	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
2	B	99	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	99	 83% 14% ..
2	F	99	 85% 14% .
2	H	99	 74% 23% ..
3	M	8	 88% 13%
3	N	8	 50% 50%
3	O	8	 88% 13%
3	P	8	 75% 25%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12321 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2192	1389	379	415	9			
1	E	277	Total	C	N	O	S	0	2	0
			2216	1409	383	415	9			
1	C	277	Total	C	N	O	S	0	0	0
			2166	1375	370	413	8			
1	G	277	Total	C	N	O	S	0	0	0
			2151	1367	362	414	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	98	Total	C	N	O	S	0	0	0
			791	506	131	147	7			
2	F	98	Total	C	N	O	S	0	0	0
			799	511	134	147	7			
2	B	98	Total	C	N	O	S	0	0	0
			795	507	132	149	7			
2	D	98	Total	C	N	O	S	0	0	0
			794	508	132	147	7			

- Molecule 3 is a protein called 8-mer peptide from spike glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	8	Total	C	N	O	0	0	0
			67	46	10	11			
3	N	8	Total	C	N	O	0	0	0
			68	47	10	11			
3	O	8	Total	C	N	O	0	0	0
			66	46	9	11			
3	P	8	Total	C	N	O	0	0	0
			67	46	10	11			

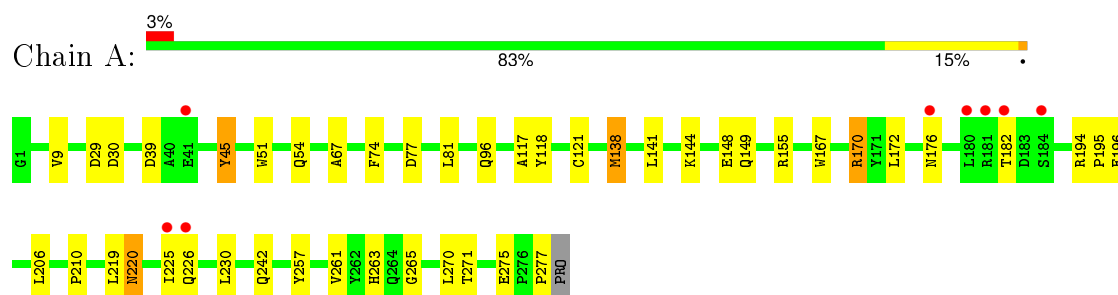
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	E	33	Total 33	O 33	0	0
4	C	13	Total 13	O 13	0	0
4	G	14	Total 14	O 14	0	0
4	H	14	Total 14	O 14	0	0
4	F	20	Total 20	O 20	0	0
4	B	13	Total 13	O 13	0	0
4	D	13	Total 13	O 13	0	0
4	M	1	Total 1	O 1	0	0
4	N	3	Total 3	O 3	0	0
4	O	2	Total 2	O 2	0	0

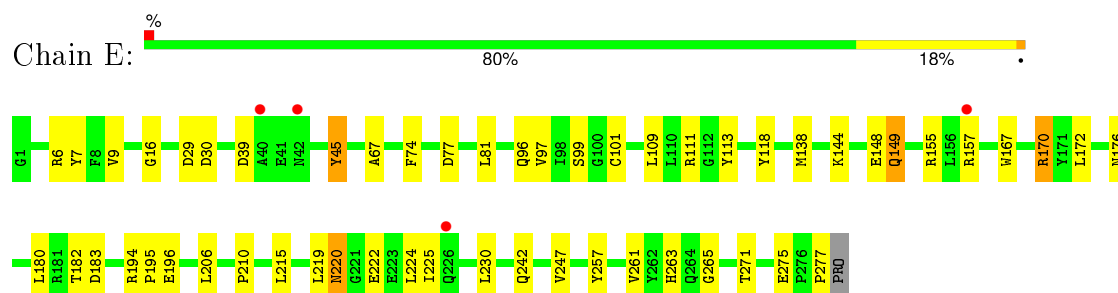
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

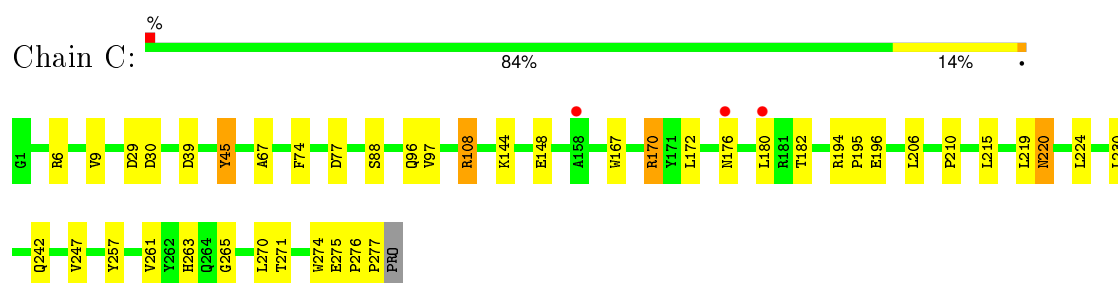
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



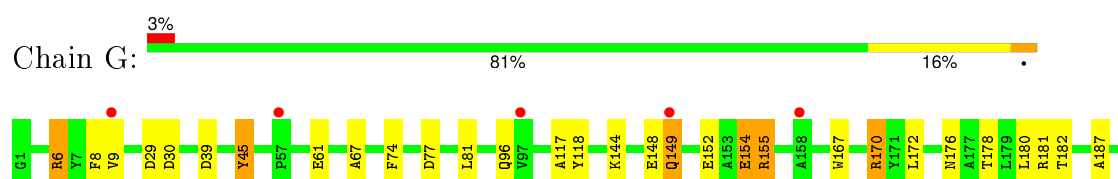
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

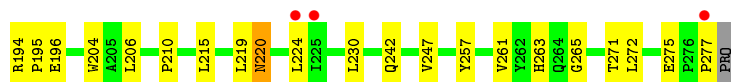


- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain





- Molecule 2: Beta-2-microglobulin

Chain H: 74% 23% ..



- Molecule 2: Beta-2-microglobulin

Chain F: 85% 14% .



- Molecule 2: Beta-2-microglobulin

Chain B: 81% 17% ..



- Molecule 2: Beta-2-microglobulin

Chain D: 83% 14% ..



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain M: 88% 13%



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain N: 50% 50%



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain O: 88% 13%



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain P:  75% 25%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.71Å 90.15Å 91.97Å 81.11° 70.58° 68.25°	Depositor
Resolution (Å)	27.00 – 2.80 26.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (27.00-2.80) 95.0 (26.86-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.253 0.212 , 0.252	Depositor DCC
$R_{free}$ test set	2240 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.4	EDS
Estimated twinning fraction	0.011 for h,h-l,k 0.011 for h,l,h-k 0.078 for h,h-k,h-l 0.089 for -h,-h+k,-l 0.058 for -h,-k,-h+l 0.020 for -h,-h+l,-h+k 0.014 for -h,-l,-k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44262 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ABA

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	0.67	1/2254 (0.0%)	0.68	1/3075 (0.0%)
1	C	0.63	0/2228	0.69	0/3042
1	E	0.65	0/2285	0.69	0/3112
1	G	0.62	0/2213	0.78	3/3024 (0.1%)
2	B	0.66	0/821	0.70	0/1118
2	D	0.65	0/820	0.70	0/1116
2	F	0.76	0/825	0.72	0/1121
2	H	0.71	0/817	0.72	0/1113
3	M	0.59	0/61	0.58	0/78
3	N	0.68	0/62	0.62	0/79
3	O	0.55	0/60	0.59	0/77
3	P	0.58	0/61	0.60	0/78
All	All	0.66	1/12507 (0.0%)	0.71	4/17033 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CYS	CB-SG	-5.74	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	155	ARG	NE-CZ-NH1	-16.60	112.00	120.30
1	G	155	ARG	NE-CZ-NH2	15.92	128.26	120.30
1	G	155	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	155	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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	2192	0	2034	25	0
1	C	2166	0	1985	27	0
1	E	2216	0	2079	31	0
1	G	2151	0	1948	33	0
2	B	795	0	735	12	0
2	D	794	0	737	10	0
2	F	799	0	753	8	0
2	H	791	0	728	14	0
3	M	67	0	67	0	0
3	N	68	0	68	2	0
3	O	66	0	65	0	0
3	P	67	0	67	1	0
4	A	23	0	0	0	0
4	B	13	0	0	0	0
4	C	13	0	0	0	0
4	D	13	0	0	2	0
4	E	33	0	0	3	0
4	F	20	0	0	0	0
4	G	14	0	0	0	0
4	H	14	0	0	0	0
4	M	1	0	0	0	0
4	N	3	0	0	1	0
4	O	2	0	0	0	0
All	All	12321	0	11266	157	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 7.

All (157) 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:108:ARG:HH21	1:C:108:ARG:HG2	1.30	0.95
2:D:73:THR:HG22	2:D:74:GLU:N	1.96	0.80
2:F:73:THR:HG22	2:F:74:GLU:N	1.97	0.79
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:TRP:CZ3	1:E:170:ARG:HD3	2.24	0.73
2:B:73:THR:HG22	2:B:74:GLU:N	2.04	0.71
1:E:6[A]:ARG:HD3	4:E:291:HOH:O	1.94	0.67
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.31	0.66
2:H:73:THR:HG22	2:H:74:GLU:N	2.10	0.66
1:G:275:GLU:O	1:G:277:PRO:HD3	1.96	0.66
2:F:73:THR:HG22	2:F:75:THR:H	1.61	0.65
1:G:167:TRP:CZ3	1:G:170:ARG:HD3	2.33	0.64
2:B:73:THR:HG22	2:B:75:THR:H	1.62	0.63
1:G:155:ARG:NH1	3:P:4:ILE:O	2.25	0.63
2:F:73:THR:CG2	2:F:74:GLU:N	2.61	0.63
1:C:108:ARG:NH2	1:C:108:ARG:HG2	2.02	0.63
1:A:149:GLN:HA	1:G:149:GLN:O	1.99	0.62
1:G:144:LYS:O	1:G:148:GLU:HG2	2.00	0.60
1:E:6[B]:ARG:HD2	1:E:113:TYR:CE1	2.36	0.60
1:G:195:PRO:O	1:G:196:GLU:HG2	2.02	0.59
1:E:275:GLU:O	1:E:277:PRO:HD3	2.03	0.58
1:G:6:ARG:NH2	1:G:6:ARG:HB2	2.18	0.58
2:H:73:THR:HG22	2:H:75:THR:H	1.69	0.58
2:D:73:THR:HG22	2:D:74:GLU:H	1.67	0.57
1:C:195:PRO:O	1:C:196:GLU:HG2	2.04	0.57
1:A:172:LEU:O	1:A:176:ASN:HB2	2.05	0.57
1:E:263:HIS:CD2	1:E:265:GLY:H	2.23	0.56
1:E:149:GLN:O	1:E:149:GLN:HG3	2.05	0.56
2:F:73:THR:HG22	2:F:74:GLU:H	1.69	0.56
1:E:263:HIS:HD2	1:E:265:GLY:H	1.53	0.56
1:A:74:PHE:HA	1:A:77:ASP:HB2	1.88	0.55
1:G:215:LEU:HD21	1:G:261:VAL:HG13	1.88	0.55
2:B:73:THR:CG2	2:B:74:GLU:N	2.69	0.55
2:D:73:THR:CG2	2:D:74:GLU:N	2.64	0.54
2:D:4:THR:HB	4:D:111:HOH:O	2.07	0.54
1:E:172:LEU:O	1:E:176:ASN:HB2	2.07	0.54
1:A:275:GLU:O	1:A:277:PRO:HD3	2.07	0.54
1:G:154:GLU:N	1:G:154:GLU:CD	2.61	0.53
1:A:194:ARG:O	1:A:195:PRO:C	2.46	0.53
1:A:195:PRO:O	1:A:196:GLU:HG2	2.09	0.53
1:C:74:PHE:HA	1:C:77:ASP:HB2	1.89	0.53
1:E:195:PRO:O	1:E:196:GLU:HG2	2.09	0.53
1:A:138:MET:HA	1:A:141:LEU:HD12	1.90	0.53
1:G:172:LEU:O	1:G:176:ASN:HB2	2.08	0.53
1:E:219:LEU:HD13	1:E:257:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HD13	1:C:257:TYR:CZ	2.44	0.52
1:G:215:LEU:CD2	1:G:261:VAL:HG13	2.39	0.52
1:E:144:LYS:O	1:E:148:GLU:HG2	2.09	0.52
1:A:206:LEU:HD23	1:A:242:GLN:HB2	1.92	0.52
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.45	0.52
2:F:73:THR:CG2	2:F:74:GLU:H	2.22	0.52
2:F:59:ASP:O	2:F:60:TRP:HB2	2.10	0.52
1:A:144:LYS:O	1:A:148:GLU:HG2	2.10	0.51
1:G:219:LEU:HD13	1:G:257:TYR:CZ	2.44	0.51
1:C:263:HIS:CD2	1:C:265:GLY:H	2.28	0.51
1:C:275:GLU:O	1:C:277:PRO:HD3	2.09	0.51
1:C:108:ARG:HH21	1:C:108:ARG:CG	2.14	0.51
1:C:194:ARG:O	1:C:195:PRO:C	2.49	0.51
1:C:144:LYS:O	1:C:148:GLU:HG2	2.11	0.51
2:D:73:THR:HG22	2:D:75:THR:H	1.75	0.51
1:G:74:PHE:HA	1:G:77:ASP:HB2	1.91	0.51
1:E:16:GLY:N	4:E:305:HOH:O	2.41	0.51
2:H:73:THR:CG2	2:H:74:GLU:N	2.74	0.50
1:A:225:ILE:HG23	1:A:226:GLN:H	1.76	0.50
1:C:261:VAL:HB	1:C:270:LEU:HB2	1.93	0.50
3:N:7:ASN:OD1	4:N:15:HOH:O	2.20	0.50
1:C:263:HIS:HD2	1:C:265:GLY:H	1.60	0.50
1:G:29:ASP:O	1:G:30:ASP:HB2	2.11	0.50
1:C:210:PRO:O	1:C:263:HIS:HE1	1.95	0.49
1:C:172:LEU:O	1:C:176:ASN:HB2	2.12	0.49
2:D:6:GLN:NE2	4:D:111:HOH:O	2.40	0.49
2:D:59:ASP:O	2:D:60:TRP:HB2	2.13	0.49
1:G:194:ARG:O	1:G:195:PRO:C	2.50	0.49
1:G:195:PRO:C	1:G:196:GLU:HG2	2.32	0.49
1:A:263:HIS:HD2	1:A:265:GLY:H	1.61	0.49
1:E:194:ARG:O	1:E:195:PRO:C	2.50	0.48
1:C:29:ASP:O	1:C:30:ASP:HB2	2.13	0.48
1:A:263:HIS:CD2	1:A:265:GLY:H	2.31	0.48
1:A:45:TYR:HE1	1:A:67:ALA:HB2	1.79	0.48
1:C:206:LEU:HD23	1:C:242:GLN:HB2	1.95	0.48
1:G:45:TYR:HE1	1:G:67:ALA:HB2	1.79	0.47
1:E:215:LEU:CD2	1:E:261:VAL:HG13	2.44	0.47
1:E:111:ARG:HG2	1:E:111:ARG:HH11	1.79	0.47
1:E:74:PHE:HA	1:E:77:ASP:HB2	1.96	0.47
2:H:17:ASN:OD1	2:H:97:ARG:NH1	2.48	0.47
2:H:16:GLU:OE2	2:H:19:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG23	1:A:226:GLN:N	2.30	0.46
1:E:215:LEU:HD21	1:E:261:VAL:HG13	1.96	0.46
2:B:55:SER:HB2	2:B:63:TYR:CE2	2.50	0.46
2:D:73:THR:CG2	2:D:74:GLU:H	2.27	0.46
2:H:39:MET:O	2:H:46:ILE:HG13	2.16	0.46
2:B:73:THR:HG22	2:B:74:GLU:H	1.77	0.46
1:G:263:HIS:CD2	1:G:265:GLY:H	2.34	0.45
1:G:187:ALA:HA	1:G:204:TRP:O	2.16	0.45
1:C:45:TYR:HE1	1:C:67:ALA:HB2	1.80	0.45
1:G:206:LEU:HD23	1:G:242:GLN:HB2	1.98	0.45
1:G:152:GLU:OE2	1:G:155:ARG:NH2	2.47	0.45
1:C:195:PRO:C	1:C:196:GLU:HG2	2.36	0.45
1:C:9:VAL:HB	1:C:97:VAL:HB	1.98	0.45
1:G:263:HIS:HD2	1:G:265:GLY:H	1.64	0.45
1:E:7:TYR:N	1:E:99:SER:O	2.46	0.45
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.98	0.45
1:E:29:ASP:O	1:E:30:ASP:HB2	2.16	0.45
2:H:59:ASP:O	2:H:60:TRP:HB2	2.17	0.45
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.52	0.44
2:D:55:SER:HB2	2:D:63:TYR:CE2	2.52	0.44
1:C:274:TRP:CD1	1:C:276:PRO:HD3	2.53	0.44
1:E:195:PRO:C	1:E:196:GLU:HG2	2.37	0.44
1:A:210:PRO:O	1:A:263:HIS:HE1	2.01	0.44
1:G:224:LEU:HD13	1:G:247:VAL:HG21	1.99	0.44
2:H:55:SER:HB2	2:H:63:TYR:CE2	2.53	0.44
1:E:224:LEU:HD13	1:E:247:VAL:HG21	1.99	0.44
1:C:170:ARG:HH11	1:C:170:ARG:HG3	1.82	0.44
1:E:215:LEU:HD22	1:E:261:VAL:HG22	1.98	0.44
1:E:9:VAL:HB	1:E:97:VAL:HB	1.99	0.44
1:E:206:LEU:HD23	1:E:242:GLN:HB2	2.00	0.44
1:G:210:PRO:O	1:G:263:HIS:HE1	2.01	0.44
1:A:29:ASP:O	1:A:30:ASP:HB2	2.17	0.44
2:B:39:MET:O	2:B:46:ILE:HG13	2.18	0.44
2:H:4:THR:HA	2:H:5:PRO:HD3	1.86	0.44
1:A:138:MET:HG2	1:A:138:MET:H	1.64	0.43
1:G:81:LEU:HD13	1:G:118:TYR:CD1	2.53	0.43
1:E:210:PRO:O	1:E:263:HIS:HE1	2.00	0.43
1:A:195:PRO:C	1:A:196:GLU:HG2	2.38	0.43
1:C:170:ARG:NH1	1:C:170:ARG:HG3	2.33	0.43
1:C:215:LEU:HD22	1:C:261:VAL:HG22	2.00	0.43
1:E:101:CYS:HB2	1:E:109:LEU:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ASP:O	2:B:60:TRP:HB2	2.18	0.43
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.54	0.43
2:F:39:MET:O	2:F:46:ILE:HG13	2.19	0.43
2:F:19:LYS:O	2:F:72:PRO:HD2	2.19	0.43
1:E:81:LEU:HD13	1:E:118:TYR:CD1	2.54	0.43
2:B:25:CYS:HB3	2:B:66:ALA:HB3	1.99	0.43
1:C:224:LEU:HD13	1:C:247:VAL:HG21	2.00	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.42
1:G:8:PHE:CD2	2:H:56:PHE:CE2	3.07	0.42
2:H:6:GLN:HG2	2:H:29:GLN:HG3	2.01	0.42
1:C:215:LEU:CD2	1:C:261:VAL:HG13	2.49	0.42
1:C:9:VAL:O	1:C:96:GLN:HA	2.19	0.42
1:E:45:TYR:HE1	1:E:67:ALA:HB2	1.84	0.42
2:H:24:ASN:HB3	2:H:65:LEU:HD11	2.01	0.42
2:B:73:THR:CG2	2:B:74:GLU:H	2.32	0.42
2:D:39:MET:O	2:D:46:ILE:HG13	2.20	0.42
1:A:9:VAL:O	1:A:96:GLN:HA	2.20	0.42
1:G:61:GLU:OE1	1:G:61:GLU:HA	2.21	0.41
1:E:155:ARG:CZ	3:N:3:TYR:OH	2.68	0.41
1:G:178:THR:O	1:G:181:ARG:HB3	2.21	0.41
2:H:25:CYS:HB3	2:H:66:ALA:HB3	2.03	0.41
1:E:183:ASP:HA	4:E:299:HOH:O	2.20	0.41
1:G:170:ARG:NH1	1:G:170:ARG:HG3	2.35	0.41
1:G:9:VAL:O	1:G:96:GLN:HA	2.21	0.41
2:B:19:LYS:O	2:B:72:PRO:HD2	2.20	0.41
2:B:4:THR:HA	2:B:5:PRO:HD3	1.88	0.40
1:A:51:TRP:O	1:A:54:GLN:HG3	2.21	0.40
1:G:154:GLU:CD	1:G:154:GLU:H	2.25	0.40
1:E:9:VAL:O	1:E:96:GLN:HA	2.21	0.40
1:G:215:LEU:HD22	1:G:261:VAL:HG22	2.03	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	275/278 (99%)	263 (96%)	11 (4%)	1 (0%)	39	74
1	C	275/278 (99%)	265 (96%)	9 (3%)	1 (0%)	39	74
1	E	277/278 (100%)	264 (95%)	12 (4%)	1 (0%)	39	74
1	G	275/278 (99%)	263 (96%)	11 (4%)	1 (0%)	39	74
2	B	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
2	D	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
2	F	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
2	H	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
3	M	5/8 (62%)	5 (100%)	0	0	100	100
3	N	5/8 (62%)	5 (100%)	0	0	100	100
3	O	5/8 (62%)	5 (100%)	0	0	100	100
3	P	5/8 (62%)	5 (100%)	0	0	100	100
All	All	1506/1540 (98%)	1445 (96%)	57 (4%)	4 (0%)	46	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	E	220	ASN
1	C	220	ASN
1	G	220	ASN

### 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	220/236 (93%)	212 (96%)	8 (4%)	42	76
1	C	213/236 (90%)	202 (95%)	11 (5%)	29	62
1	E	223/236 (94%)	210 (94%)	13 (6%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	209/236 (89%)	197 (94%)	12 (6%)	25	58
2	B	87/94 (93%)	83 (95%)	4 (5%)	33	67
2	D	86/94 (92%)	79 (92%)	7 (8%)	15	39
2	F	88/94 (94%)	83 (94%)	5 (6%)	25	58
2	H	85/94 (90%)	80 (94%)	5 (6%)	24	57
3	M	5/6 (83%)	4 (80%)	1 (20%)	1	5
3	N	6/6 (100%)	4 (67%)	2 (33%)	0	1
3	O	5/6 (83%)	4 (80%)	1 (20%)	1	5
3	P	5/6 (83%)	4 (80%)	1 (20%)	1	5
All	All	1232/1344 (92%)	1162 (94%)	70 (6%)	25	58

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	45	TYR
1	A	138	MET
1	A	170	ARG
1	A	182	THR
1	A	220	ASN
1	A	230	LEU
1	A	271	THR
1	E	39	ASP
1	E	45	TYR
1	E	138	MET
1	E	149	GLN
1	E	157	ARG
1	E	170	ARG
1	E	180	LEU
1	E	182	THR
1	E	220	ASN
1	E	222	GLU
1	E	225	ILE
1	E	230	LEU
1	E	271	THR
1	C	6	ARG
1	C	39	ASP
1	C	45	TYR
1	C	88	SER

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Mol	Chain	Res	Type
1	C	108	ARG
1	C	170	ARG
1	C	180	LEU
1	C	182	THR
1	C	220	ASN
1	C	230	LEU
1	C	271	THR
1	G	6	ARG
1	G	39	ASP
1	G	45	TYR
1	G	149	GLN
1	G	154	GLU
1	G	170	ARG
1	G	180	LEU
1	G	182	THR
1	G	220	ASN
1	G	230	LEU
1	G	271	THR
1	G	272	LEU
2	H	4	THR
2	H	50	GLU
2	H	54	MET
2	H	70	PHE
2	H	97	ARG
2	F	4	THR
2	F	50	GLU
2	F	54	MET
2	F	70	PHE
2	F	97	ARG
2	B	4	THR
2	B	50	GLU
2	B	54	MET
2	B	70	PHE
2	D	4	THR
2	D	19	LYS
2	D	50	GLU
2	D	54	MET
2	D	55	SER
2	D	70	PHE
2	D	97	ARG
3	M	8	ILE
3	N	1	ARG

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Mol	Chain	Res	Type
3	N	8	ILE
3	O	8	ILE
3	P	8	ILE

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	220	ASN
1	A	263	HIS
1	E	263	HIS
1	C	220	ASN
1	C	263	HIS
1	G	263	HIS
3	N	7	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ABA	M	2	3	4,5,6	0.51	0	3,5,7	1.13	0
3	ABA	N	2	3	4,5,6	0.59	0	3,5,7	1.18	1 (33%)
3	ABA	O	2	3	4,5,6	0.45	0	3,5,7	1.12	0
3	ABA	P	2	3	4,5,6	0.46	0	3,5,7	1.19	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ABA	M	2	3	-	0/2/4/6	0/0/0/0
3	ABA	N	2	3	-	0/2/4/6	0/0/0/0
3	ABA	O	2	3	-	0/2/4/6	0/0/0/0
3	ABA	P	2	3	-	0/2/4/6	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	2	ABA	O-C-CA	-2.04	120.17	125.49
3	P	2	ABA	O-C-CA	-2.04	120.19	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/278 (99%)	-0.11	8 (2%) 55 43	38, 42, 45, 49	0
1	C	277/278 (99%)	-0.15	3 (1%) 82 74	37, 42, 45, 48	0
1	E	277/278 (99%)	-0.10	4 (1%) 78 69	37, 42, 45, 46	0
1	G	277/278 (99%)	-0.04	8 (2%) 55 43	40, 42, 45, 49	0
2	B	98/99 (98%)	-0.47	0 100 100	40, 42, 44, 45	0
2	D	98/99 (98%)	-0.37	0 100 100	40, 42, 44, 45	0
2	F	98/99 (98%)	-0.52	0 100 100	40, 42, 44, 46	0
2	H	98/99 (98%)	-0.52	0 100 100	40, 42, 44, 45	0
3	M	7/8 (87%)	-0.41	0 100 100	41, 42, 43, 43	0
3	N	7/8 (87%)	-0.37	0 100 100	41, 42, 43, 43	0
3	O	7/8 (87%)	-0.56	0 100 100	41, 42, 43, 43	0
3	P	7/8 (87%)	-0.42	0 100 100	41, 42, 43, 43	0
All	All	1528/1540 (99%)	-0.20	23 (1%) 76 68	37, 42, 45, 49	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	LEU	3.8
1	G	149	GLN	3.5
1	A	180	LEU	3.0
1	A	226	GLN	2.8
1	G	277	PRO	2.7
1	E	42	ASN	2.7
1	E	40	ALA	2.7
1	G	158	ALA	2.6
1	A	225	ILE	2.6
1	C	176	ASN	2.3
1	E	226	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	157	ARG	2.2
1	A	184	SER	2.1
1	A	176	ASN	2.1
1	A	182	THR	2.1
1	G	9	VAL	2.1
1	C	158	ALA	2.1
1	G	57	PRO	2.1
1	G	97	VAL	2.1
1	G	225	ILE	2.0
1	A	181	ARG	2.0
1	G	224	LEU	2.0
1	A	41	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ABA	O	2	6/7	0.97	0.17	-	41,42,42,42	0
3	ABA	N	2	6/7	0.96	0.18	-	41,42,42,42	0
3	ABA	P	2	6/7	0.97	0.19	-	41,42,42,42	0
3	ABA	M	2	6/7	0.96	0.18	-	41,42,42,42	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.