Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2016 – 01:34 PM EST

PDB ID	:	5GGS
Title	:	PD-1 in complex with pembrolizumab Fab
Authors	:	Heo, Y.S.
Deposited on	:	2016-06-16
Resolution	:	2.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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)	:	rb-20028320

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 2.00 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		1.4%
RSRZ outliers		5.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
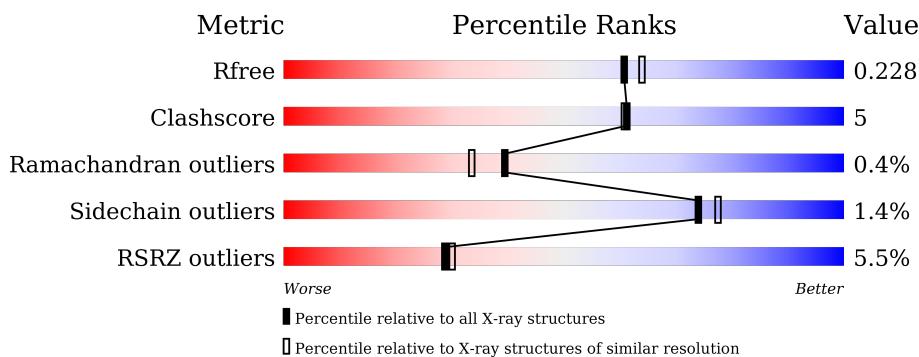
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	232	.% / 84% 10% · 6%
1	C	232	2% / 83% 11% · 5%
2	B	218	2% / 90% 10%
2	D	218	2% / 91% 8%
3	Y	123	20% / 78% 13% · 7%
3	Z	123	18% / 73% 15% ·· 8%
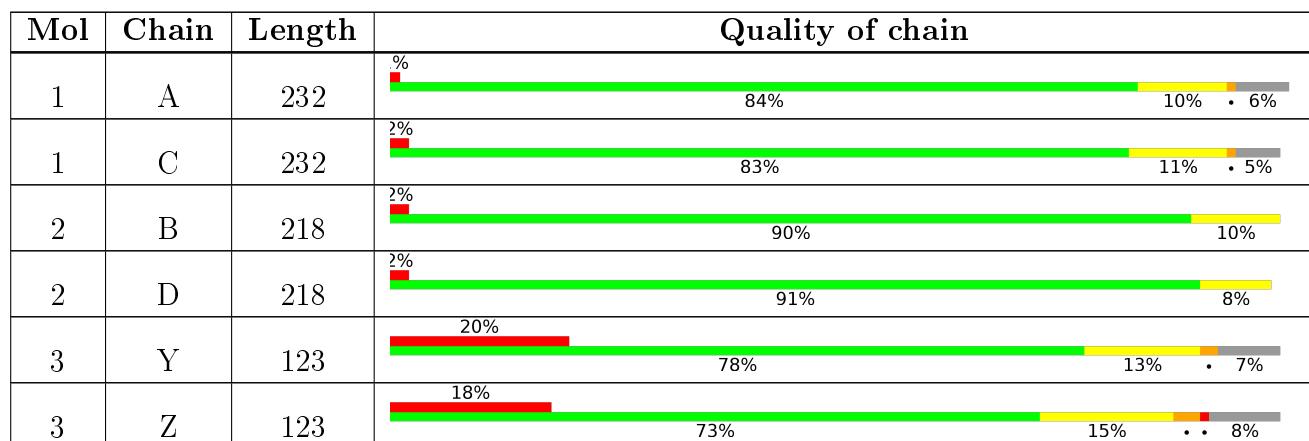
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9239 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total 1660	C 1050	N 274	O 328	S 8	0	0	0
1	C	220	Total 1669	C 1055	N 276	O 330	S 8	0	0	0

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total 1666	C 1048	N 279	O 335	S 4	0	0	0
2	D	217	Total 1666	C 1048	N 279	O 335	S 4	0	0	0

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	114	Total 892	C 552	N 162	O 174	S 4	0	0	0
3	Z	113	Total 890	C 554	N 162	O 170	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	93	SER	CYS	engineered mutation	UNP Q15116
Z	93	SER	CYS	engineered mutation	UNP Q15116

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total 147	O 147	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	203	Total 203	O 203	0	0
4	C	168	Total 168	O 168	0	0
4	D	196	Total 196	O 196	0	0
4	Y	43	Total 43	O 43	0	0
4	Z	39	Total 39	O 39	0	0

3 Residue-property plots ⓘ

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: heavy chain
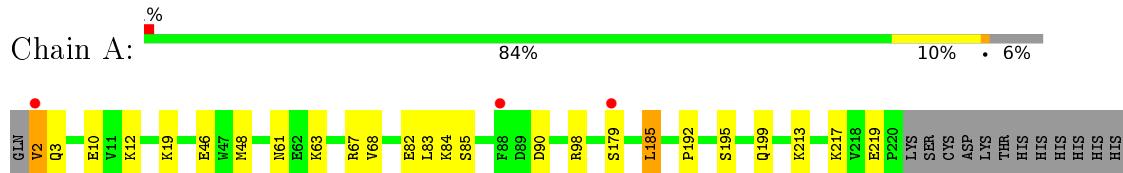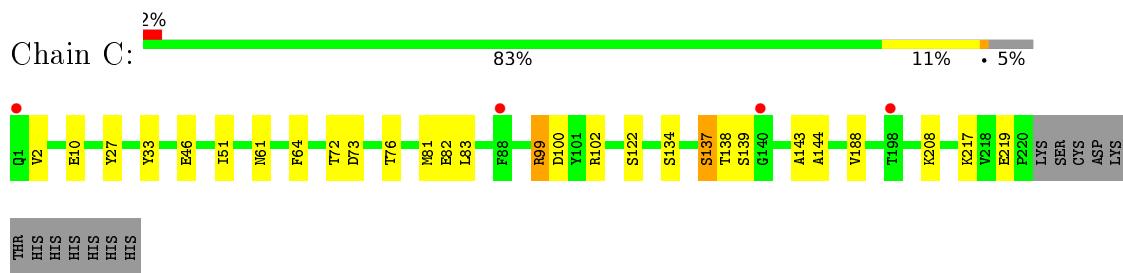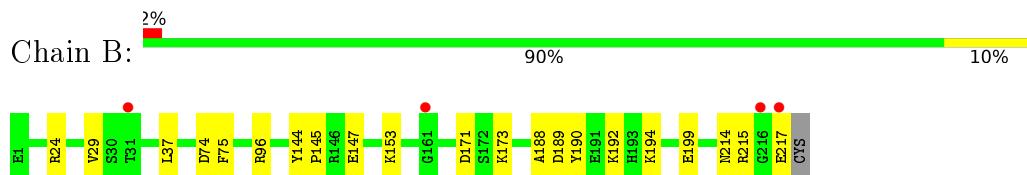
Chain A:

- Molecule 1: heavy chain

Chain C:

- Molecule 2: light chain

Chain B:

- Molecule 2: light chain

Chain D:

- Molecule 3: Programmed cell death protein 1

Chain Y:

V144 T145 E146 ARG ARG

• Molecule 3: Programmed cell death protein 1

Chain Z:

18%

73%

15%

8%

ASP SER PRO ASP ARG P31 S38 P39 A40 L41 L42 V43 V44 T45 E46 G47 D48 S57 N58 T59 S60 E61 S62 R69 R86 Q91 R96 R104 R112 A113 R114 R115 M116 L122 L128 A129 P130 K131 A132 Q133 R139 R143 VAL THR GLU ARG ARG
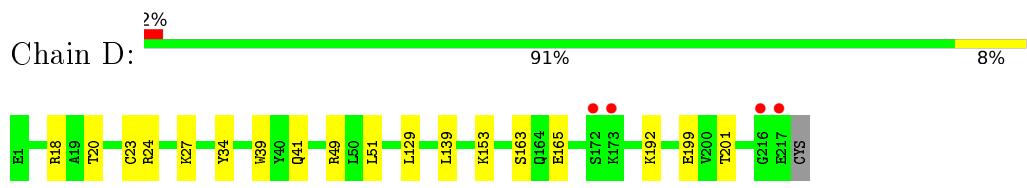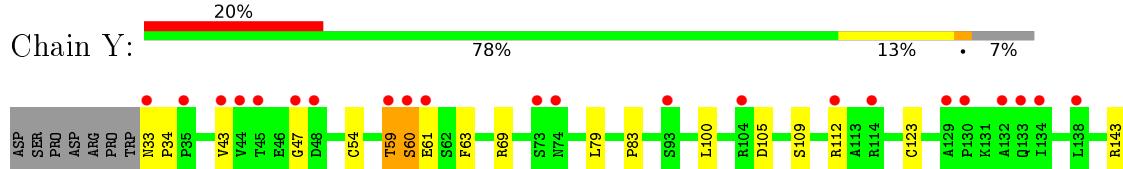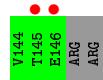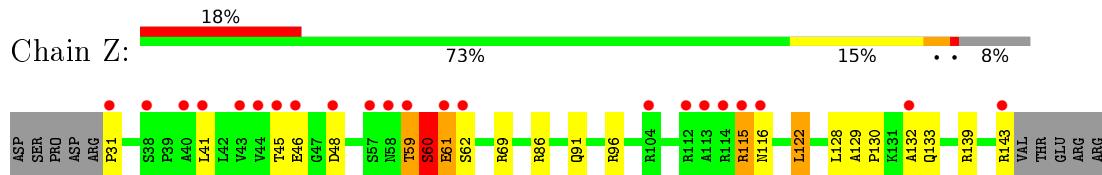
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.17Å 54.20Å 104.04Å 105.69° 96.99° 96.06°	Depositor
Resolution (Å)	30.04 – 2.00 30.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.04-2.00) 85.7 (30.04-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.179 , 0.228 0.181 , 0.228	Depositor DCC
R_{free} test set	3606 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9239	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.41	0/1702	0.56	1/2318 (0.0%)
1	C	0.42	0/1711	0.56	0/2330
2	B	0.41	0/1704	0.56	0/2315
2	D	0.42	0/1704	0.54	0/2315
3	Y	0.35	0/911	0.57	0/1236
3	Z	0.33	0/912	0.57	0/1238
All	All	0.40	0/8644	0.56	1/11752 (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
3	Z	0	1

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	A	185	LEU	CA-CB-CG	5.27	127.43	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Z	61	GLU	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	1660	0	1610	16	1
1	C	1669	0	1621	22	0
2	B	1666	0	1624	14	0
2	D	1666	0	1624	15	0
3	Y	892	0	864	12	0
3	Z	890	0	858	15	0
4	A	147	0	0	6	2
4	B	203	0	0	5	0
4	C	168	0	0	9	0
4	D	196	0	0	6	0
4	Y	43	0	0	1	0
4	Z	39	0	0	4	1
All	All	9239	0	8201	91	3

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 5.

All (91) 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:208:LYS:NZ	4:C:301:HOH:O	1.82	1.12
2:D:24:ARG:NH1	4:D:301:HOH:O	1.87	1.07
1:C:217:LYS:NZ	1:C:219:GLU:OE2	1.91	1.02
1:A:48:MET:SD	4:A:444:HOH:O	2.27	0.92
1:C:99:ARG:NE	4:C:302:HOH:O	2.04	0.89
3:Y:59:THR:OG1	3:Y:61:GLU:HG2	1.76	0.85
2:D:153:LYS:NZ	2:D:199:GLU:OE2	2.11	0.83
1:A:82:GLU:OE1	4:A:301:HOH:O	1.96	0.82
2:B:153:LYS:NZ	2:B:199:GLU:OE1	2.14	0.79
1:C:99:ARG:CZ	4:C:302:HOH:O	2.28	0.79
2:B:24:ARG:NH1	2:B:74:ASP:HB2	1.98	0.78
1:C:99:ARG:NH1	1:C:100:ASP:O	2.18	0.77
2:D:165:GLU:OE2	4:D:302:HOH:O	2.02	0.77
3:Y:59:THR:HG1	3:Y:61:GLU:HG2	1.51	0.75
1:C:139:SER:OG	4:C:303:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:LYS:NZ	4:D:304:HOH:O	2.22	0.71
1:C:188:VAL:HG21	2:D:139:LEU:HD22	1.73	0.70
2:B:217:GLU:OE2	4:B:301:HOH:O	2.12	0.67
1:C:99:ARG:NH2	4:C:302:HOH:O	2.25	0.67
1:C:82:GLU:OE1	4:C:304:HOH:O	2.13	0.66
1:A:63:LYS:NZ	4:A:305:HOH:O	2.29	0.65
1:A:19:LYS:NZ	4:A:302:HOH:O	2.17	0.64
2:B:24:ARG:HH11	2:B:74:ASP:HB2	1.62	0.63
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.28	0.63
1:C:81:MET:HE1	1:C:83:LEU:HB2	1.82	0.62
1:C:137:SER:OG	1:C:144:ALA:O	2.18	0.62
2:B:215:ARG:HD3	4:B:302:HOH:O	2.00	0.61
2:B:190:TYR:O	4:B:302:HOH:O	2.17	0.60
3:Y:143:ARG:NH2	4:Y:201:HOH:O	2.17	0.59
3:Z:62:SER:HB3	3:Z:128:LEU:HD12	1.84	0.59
2:D:49:ARG:NH2	4:D:306:HOH:O	2.35	0.58
1:C:10:GLU:OE2	4:C:305:HOH:O	2.18	0.57
2:D:18:ARG:HH11	2:D:20:THR:HG23	1.70	0.56
1:C:73:ASP:OD2	1:C:76:THR:OG1	2.12	0.56
2:D:18:ARG:HH11	2:D:20:THR:CG2	2.18	0.56
2:B:188:ALA:O	2:B:192:LYS:HG2	2.05	0.56
1:A:3:GLN:HG2	4:A:315:HOH:O	2.04	0.55
1:C:33:TYR:CD2	1:C:99:ARG:NH1	2.74	0.55
3:Y:100:LEU:HD12	3:Y:105:ASP:HB2	1.87	0.55
3:Y:61:GLU:O	3:Y:63:PHE:HD2	1.90	0.55
2:D:163:SER:OG	4:D:303:HOH:O	2.18	0.54
3:Z:122:LEU:HD22	3:Z:139:ARG:HG2	1.91	0.52
3:Z:31:PRO:HD2	4:Z:202:HOH:O	2.08	0.52
1:A:46:GLU:OE2	1:A:63:LYS:HE3	2.10	0.52
3:Z:129:ALA:HB3	3:Z:130:PRO:HD3	1.92	0.51
1:C:134:SER:O	1:C:138:THR:HG23	2.10	0.51
2:B:194:LYS:HE2	2:B:214:ASN:HB3	1.92	0.50
2:B:37:LEU:HD22	2:B:75:PHE:CG	2.47	0.50
3:Z:96:ARG:NH1	4:Z:203:HOH:O	2.44	0.50
2:B:147:GLU:HG2	2:D:201:THR:HG21	1.92	0.50
3:Y:54:CYS:HG	3:Y:123:CYS:HG	1.56	0.49
1:C:51:ILE:HD13	1:C:72:THR:HG23	1.95	0.49
1:C:134:SER:H	1:C:137:SER:HB3	1.77	0.48
2:D:27:LYS:HD2	4:D:339:HOH:O	2.12	0.48
1:A:68:VAL:HG22	1:A:83:LEU:HD13	1.96	0.48
3:Y:59:THR:OG1	3:Y:60:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:NE2	4:A:315:HOH:O	2.47	0.47
1:A:61:ASN:HD21	1:A:63:LYS:NZ	2.13	0.46
3:Z:115:ARG:HG3	3:Z:116:ASN:N	2.30	0.45
3:Z:130:PRO:O	3:Z:132:ALA:N	2.41	0.45
1:A:213:LYS:HE2	1:A:213:LYS:HB3	1.81	0.45
4:B:304:HOH:O	3:Z:86:ARG:NH1	2.46	0.44
3:Z:69:ARG:NH2	3:Z:116:ASN:O	2.49	0.44
3:Z:130:PRO:HB2	3:Z:133:GLN:HG3	1.99	0.44
1:C:46:GLU:OE1	4:C:306:HOH:O	2.21	0.44
3:Z:41:LEU:HD11	3:Z:143:ARG:NH1	2.31	0.44
1:C:102:ARG:HD3	4:C:429:HOH:O	2.17	0.43
1:A:10:GLU:OE1	1:A:12:LYS:NZ	2.51	0.43
3:Z:91:GLN:NE2	4:Z:204:HOH:O	2.50	0.43
1:A:192:PRO:HG2	1:A:195:SER:HB3	1.99	0.43
3:Z:60:SER:N	3:Z:61:GLU:HG3	2.32	0.43
2:D:129:LEU:HD23	2:D:129:LEU:HA	1.86	0.43
3:Y:33:ASN:N	3:Y:34:PRO:HD3	2.33	0.43
3:Y:43:VAL:HG12	3:Y:143:ARG:HB2	2.02	0.42
2:D:23:CYS:HB2	2:D:39:TRP:CH2	2.54	0.42
3:Z:59:THR:C	3:Z:61:GLU:HG3	2.40	0.42
1:A:2:VAL:HG21	1:A:98:ARG:HH12	1.85	0.42
2:B:171:ASP:OD2	2:B:173:LYS:HB2	2.19	0.42
2:B:29:VAL:HA	2:B:96:ARG:HG2	2.03	0.41
3:Y:47:GLY:O	3:Y:112:ARG:HA	2.19	0.41
3:Z:91:GLN:N	4:Z:206:HOH:O	2.52	0.41
2:D:41:GLN:HB2	2:D:51:LEU:HD11	2.02	0.41
1:A:217:LYS:HE2	1:A:219:GLU:HG2	2.01	0.41
2:B:144:TYR:CG	2:B:145:PRO:HA	2.56	0.41
3:Y:69:ARG:HB2	3:Y:79:LEU:HD11	2.03	0.41
1:A:82:GLU:OE2	1:A:84:LYS:HE2	2.21	0.41
2:B:189:ASP:OD2	4:B:303:HOH:O	2.21	0.41
1:C:2:VAL:HG22	1:C:27:TYR:HB3	2.02	0.41
1:C:61:ASN:HB3	1:C:64:PHE:HD2	1.86	0.41
1:C:138:THR:HG22	1:C:143:ALA:HB2	2.01	0.40
2:D:34:TYR:CD2	3:Y:83:PRO:HG3	2.56	0.40

All (3) 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)
4:A:447:HOH:O	4:Z:237:HOH:O[1_465]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:424:HOH:O	4:A:432:HOH:O[1_565]	2.11	0.09
1:A:85:SER:OG	1:A:199:GLN:OE1[1_545]	2.17	0.03

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	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	C	218/232 (94%)	214 (98%)	4 (2%)	0	100	100
2	B	215/218 (99%)	211 (98%)	4 (2%)	0	100	100
2	D	215/218 (99%)	211 (98%)	4 (2%)	0	100	100
3	Y	112/123 (91%)	105 (94%)	5 (4%)	2 (2%)	11	4
3	Z	111/123 (90%)	104 (94%)	5 (4%)	2 (2%)	11	4
All	All	1088/1146 (95%)	1059 (97%)	25 (2%)	4 (0%)	39	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	59	THR
3	Y	60	SER
3	Z	60	SER
3	Z	46	GLU

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	187/200 (94%)	184 (98%)	3 (2%)	70	73
1	C	188/200 (94%)	185 (98%)	3 (2%)	70	73
2	B	188/189 (100%)	188 (100%)	0	100	100
2	D	188/189 (100%)	188 (100%)	0	100	100
3	Y	100/109 (92%)	99 (99%)	1 (1%)	82	85
3	Z	99/109 (91%)	93 (94%)	6 (6%)	23	17
All	All	950/996 (95%)	937 (99%)	13 (1%)	74	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	179	SER
1	A	185	LEU
1	C	99	ARG
1	C	122	SER
1	C	137	SER
3	Y	109	SER
3	Z	45	THR
3	Z	48	ASP
3	Z	59	THR
3	Z	60	SER
3	Z	115	ARG
3	Z	122	LEU

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

Mol	Chain	Res	Type
1	A	61	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 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 (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(Å²)	Q<0.9
1	A	219/232 (94%)	0.10	3 (1%)	78	78	16, 25, 41, 51	0
1	C	220/232 (94%)	0.08	4 (1%)	71	72	15, 25, 46, 59	0
2	B	217/218 (99%)	0.03	4 (1%)	71	72	14, 22, 41, 50	0
2	D	217/218 (99%)	0.01	4 (1%)	71	72	14, 22, 39, 53	0
3	Y	114/123 (92%)	1.08	24 (21%)	1	1	22, 43, 74, 84	0
3	Z	113/123 (91%)	1.04	22 (19%)	1	2	22, 45, 72, 89	0
All	All	1100/1146 (95%)	0.26	61 (5%)	29	30	14, 26, 54, 89	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	59	THR	7.1
3	Z	45	THR	5.9
3	Y	129	ALA	5.7
3	Y	132	ALA	5.5
3	Z	61	GLU	5.5
3	Y	61	GLU	5.2
1	A	2	VAL	4.8
3	Z	116	ASN	4.7
3	Y	60	SER	4.5
3	Z	48	ASP	4.5
3	Z	115	ARG	4.5
3	Y	45	THR	4.3
3	Z	132	ALA	4.1
3	Y	145	THR	4.1
2	D	217	GLU	3.9
3	Z	59	THR	3.9
3	Y	74	ASN	3.7
3	Y	130	PRO	3.7
3	Z	44	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	Z	41	LEU	3.5
3	Y	133	GLN	3.5
3	Z	113	ALA	3.3
1	C	140	GLY	3.3
3	Y	138	LEU	3.1
3	Z	114	ARG	3.1
2	B	217	GLU	3.1
3	Z	46	GLU	3.1
3	Y	146	GLU	3.1
3	Y	35	PRO	2.9
3	Y	112	ARG	2.9
2	B	216	GLY	2.8
3	Y	134	ILE	2.8
3	Z	38	SER	2.8
3	Z	62	SER	2.7
3	Y	104	ARG	2.7
1	A	88	PHE	2.7
2	D	172	SER	2.7
3	Z	43	VAL	2.6
2	D	216	GLY	2.5
3	Z	58	ASN	2.5
3	Y	47	GLY	2.5
2	D	173	LYS	2.5
1	C	198	THR	2.4
3	Y	44	VAL	2.3
3	Y	93	SER	2.3
3	Z	40	ALA	2.3
3	Y	33	ASN	2.3
1	C	88	PHE	2.3
1	C	1	GLN	2.2
2	B	31	THR	2.2
3	Z	143	ARG	2.2
2	B	161	GLY	2.2
3	Z	112	ARG	2.2
3	Y	43	VAL	2.1
3	Z	31	PRO	2.1
3	Y	48	ASP	2.1
3	Y	114	ARG	2.0
3	Z	57	SER	2.0
1	A	179	SER	2.0
3	Y	73	SER	2.0
3	Z	104	ARG	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 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.