Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 03:40 PM JST

PDB ID	:	5JXE
Title	:	Human PD-1 ectodomain complexed with Pembrolizumab Fab
Authors	:	Na, Z.; Bharath, S.R.; Song, H.
Deposited on	:	2016-05-13
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:

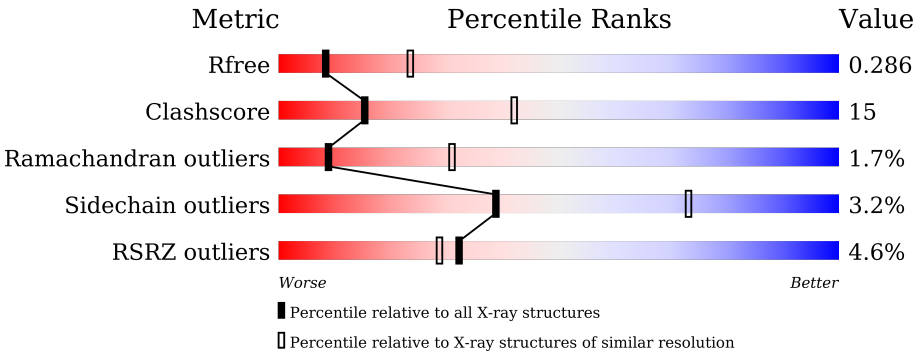
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	114	3% 53% 28% 15%
1	B	114	11% 61% 25% 11%
2	C	218	5% 62% 34%
2	F	218	3% 61% 35%
3	D	218	2% 68% 22% 10%
3	G	218	5% 79% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7851 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 Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			721	449	127	141	4			
1	B	101	Total	C	N	O	S	0	0	0
			704	448	113	140	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	SER	CYS	engineered mutation	UNP Q15116
B	93	SER	CYS	engineered mutation	UNP Q15116

- Molecule 2 is a protein called Pembrolizumab Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total	C	N	O	S	0	0	0
			1612	1015	270	323	4			
2	F	215	Total	C	N	O	S	0	0	0
			1653	1041	277	331	4			

- Molecule 3 is a protein called Pembrolizumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	197	Total	C	N	O	S	0	0	0
			1509	958	249	294	8			
3	G	218	Total	C	N	O	S	0	0	0
			1642	1036	269	328	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	O	0	0
			2	2		

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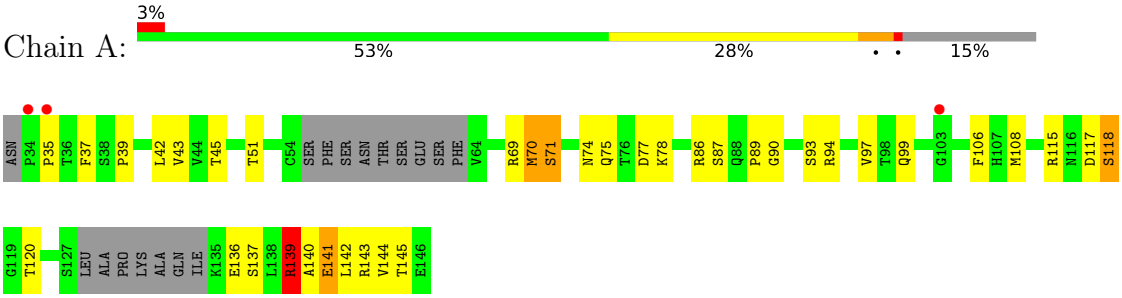
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	8	Total O 8 8	0	0

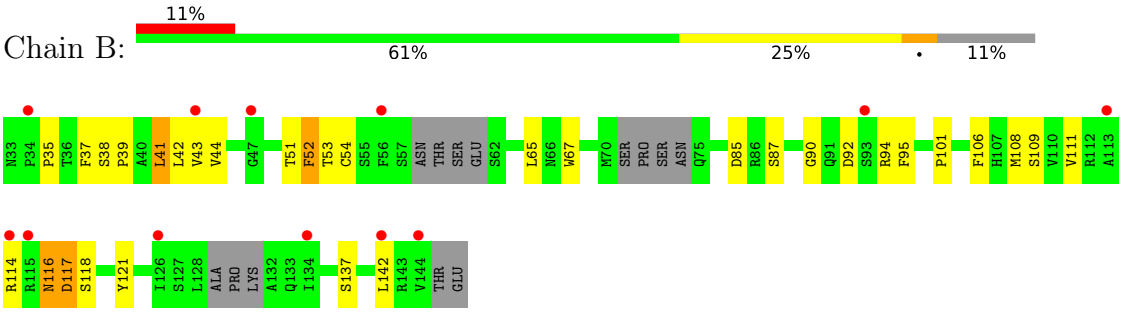
3 Residue-property plots (i)

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.

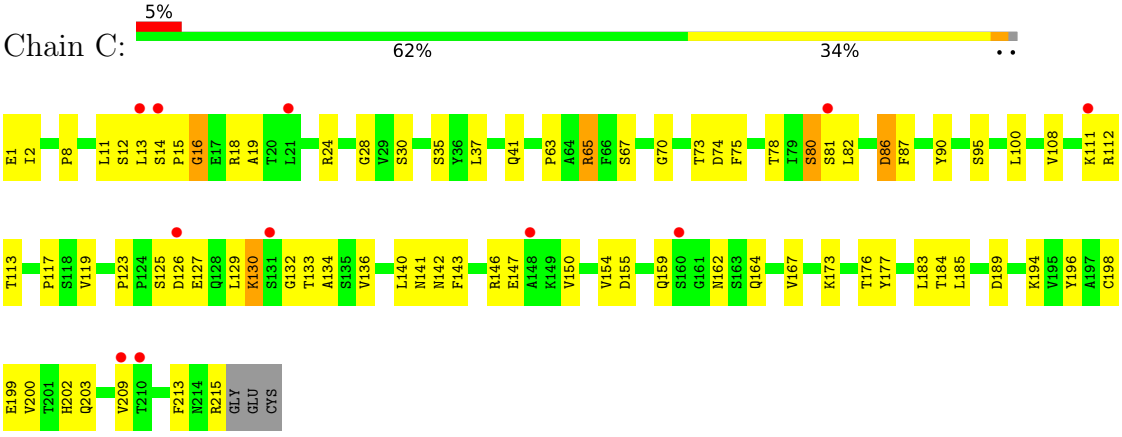
• Molecule 1: Programmed cell death protein 1



• Molecule 1: Programmed cell death protein 1

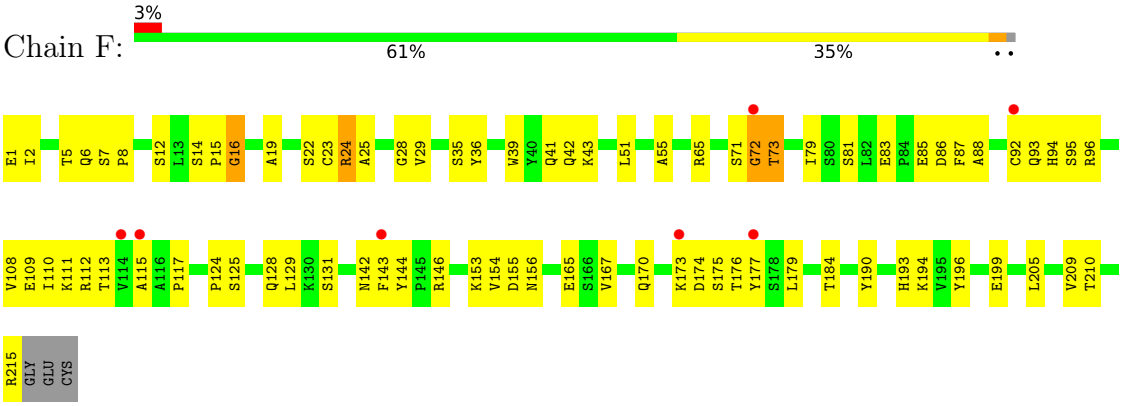


• Molecule 2: Pembrolizumab Fab light chain



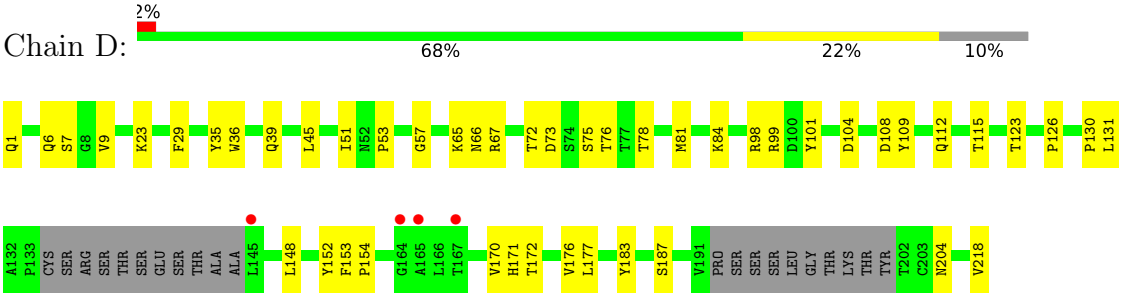
• Molecule 2: Pembrolizumab Fab light chain

Chain F:



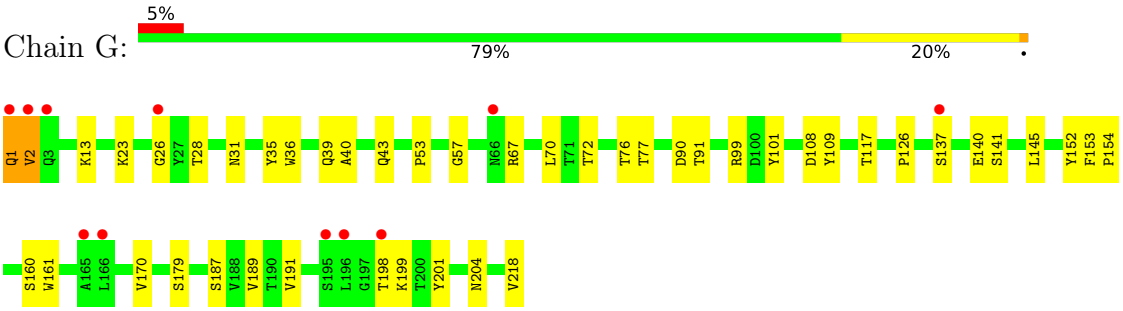
• Molecule 3: Pembrolizumab Fab heavy chain

Chain D:



• Molecule 3: Pembrolizumab Fab heavy chain

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	105.55Å 105.55Å 380.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.93 – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.93-2.90) 99.3 (29.93-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.261 , 0.286 0.261 , 0.286	Depositor DCC
R_{free} test set	1424 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.9	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	0.90	EDS
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.70	3/735 (0.4%)	0.66	1/1000 (0.1%)
1	B	0.30	0/717	0.55	0/981
2	C	0.33	0/1650	0.53	0/2252
2	F	0.31	0/1691	0.55	1/2298 (0.0%)
3	D	0.26	0/1546	0.48	0/2103
3	G	0.30	0/1683	0.48	0/2297
All	All	0.35	3/8022 (0.0%)	0.53	2/10931 (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	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ARG	CZ-NH2	-11.20	1.18	1.33
1	A	139	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	139	ARG	NE-CZ	-6.94	1.24	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	GLU	OE1-CD-OE2	-7.19	114.68	123.30
2	F	24	ARG	NE-CZ-NH1	7.01	123.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	137	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	721	0	661	34	0
1	B	704	0	613	25	0
2	C	1612	0	1525	58	0
2	F	1653	0	1615	66	0
3	D	1509	0	1452	29	0
3	G	1642	0	1565	27	0
4	D	2	0	0	0	0
4	G	8	0	0	0	0
All	All	7851	0	7431	228	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 15.

All (228) 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)
2:F:153:LYS:NZ	2:F:156:ASN:HA	1.54	1.21
2:F:153:LYS:NZ	2:F:156:ASN:OD1	1.84	1.10
1:A:120:THR:HA	1:A:139:ARG:NH2	1.70	1.07
2:F:153:LYS:CE	2:F:156:ASN:HA	1.88	1.03
2:F:153:LYS:NZ	2:F:156:ASN:CA	2.23	1.01
2:F:153:LYS:HZ3	2:F:156:ASN:CA	1.76	0.99
2:F:153:LYS:HZ3	2:F:156:ASN:N	1.61	0.97
2:C:13:LEU:HD11	2:C:82:LEU:HD22	1.41	0.97
3:G:161:TRP:HE1	3:G:187:SER:HG	1.22	0.88
1:A:141:GLU:OE1	1:A:143:ARG:NH2	2.06	0.87
1:A:120:THR:HA	1:A:139:ARG:HH22	1.36	0.86
1:B:116:ASN:O	1:B:118:SER:N	2.11	0.83
2:F:146:ARG:HD2	2:F:167:VAL:HG11	1.59	0.82
2:F:153:LYS:HZ1	2:F:156:ASN:HA	1.46	0.80
2:F:153:LYS:HE2	2:F:156:ASN:HA	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:TYR:HD2	1:B:142:LEU:HD13	1.49	0.78
2:C:28:GLY:HA2	2:C:73:THR:HA	1.66	0.77
2:F:170:GLN:NE2	2:F:175:SER:OG	2.19	0.76
2:F:153:LYS:HZ3	2:F:156:ASN:H	1.31	0.75
2:F:112:ARG:NH1	2:F:113:THR:O	2.21	0.74
3:G:160:SER:OG	3:G:204:ASN:OD1	2.06	0.73
2:F:42:GLN:HE22	3:G:39:GLN:HE22	1.35	0.72
3:G:170:VAL:HG22	3:G:189:VAL:HG22	1.72	0.72
2:C:65:ARG:NH1	2:C:86:ASP:OD2	2.23	0.71
1:B:90:GLY:HA3	3:D:57:GLY:HA3	1.73	0.70
1:B:121:TYR:CD2	1:B:142:LEU:HD13	2.27	0.69
2:C:86:ASP:O	2:C:90:TYR:OH	2.11	0.69
2:C:154:VAL:HG22	2:C:196:TYR:HD2	1.58	0.69
3:G:23:LYS:NZ	3:G:76:THR:O	2.25	0.68
1:B:87:SER:O	3:D:35:TYR:OH	2.12	0.67
2:F:128:GLN:O	2:F:131:SER:OG	2.09	0.67
2:F:155:ASP:HB2	2:F:193:HIS:HD2	1.59	0.67
1:A:87:SER:O	3:G:35:TYR:OH	2.08	0.66
2:C:73:THR:HG23	2:C:74:ASP:OD2	1.95	0.66
2:C:112:ARG:NH1	2:C:113:THR:O	2.26	0.66
3:D:51:ILE:HD13	3:D:72:THR:HG23	1.76	0.66
2:C:73:THR:HG23	2:C:74:ASP:CG	2.17	0.65
1:A:35:PRO:HG2	1:A:137:SER:HB2	1.78	0.65
2:C:18:ARG:HB2	2:C:80:SER:HA	1.79	0.65
3:G:1:GLN:N	3:G:26:GLY:HA3	2.11	0.65
3:D:73:ASP:OD2	3:D:75:SER:OG	2.14	0.65
1:B:39:PRO:HD2	1:B:42:LEU:HD21	1.78	0.65
1:A:78:LYS:NZ	3:G:101:TYR:O	2.26	0.64
2:F:71:SER:O	2:F:73:THR:N	2.31	0.64
2:F:194:LYS:NZ	2:F:215:ARG:O	2.29	0.64
3:D:126:PRO:HB3	3:D:152:TYR:HB3	1.80	0.63
3:D:99:ARG:HD3	3:D:104:ASP:HA	1.79	0.63
2:C:8:PRO:HD2	2:C:11:LEU:HD11	1.80	0.63
2:F:109:GLU:OE2	2:F:144:TYR:HE1	1.82	0.63
2:C:141:ASN:OD1	2:C:142:ASN:ND2	2.33	0.62
1:A:139:ARG:CZ	1:A:141:GLU:HG2	2.30	0.61
1:B:116:ASN:OD1	1:B:117:ASP:N	2.32	0.61
3:G:1:GLN:H3	3:G:26:GLY:HA3	1.65	0.61
3:D:6:GLN:H	3:D:112:GLN:HE22	1.47	0.61
2:C:63:PRO:HG2	2:C:65:ARG:NH2	2.15	0.60
1:B:41:LEU:O	1:B:42:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:PRO:HD3	2:C:202:HIS:CD2	2.36	0.60
2:F:174:ASP:OD2	2:F:176:THR:N	2.20	0.59
1:B:117:ASP:O	1:B:121:TYR:OH	2.13	0.59
2:F:71:SER:OG	2:F:72:GLY:N	2.35	0.59
2:F:117:PRO:HB3	2:F:143:PHE:HB3	1.83	0.59
2:F:174:ASP:OD2	2:F:176:THR:HG22	2.02	0.59
1:A:42:LEU:O	1:A:142:LEU:HA	2.02	0.59
1:A:39:PRO:O	1:A:140:ALA:HB1	2.02	0.59
1:A:120:THR:CA	1:A:139:ARG:NH2	2.57	0.59
2:F:14:SER:O	2:F:16:GLY:N	2.34	0.59
3:G:91:THR:HG23	3:G:117:THR:HA	1.84	0.58
2:C:117:PRO:HB3	2:C:143:PHE:HB3	1.86	0.58
2:F:19:ALA:HB3	2:F:79:ILE:HB	1.86	0.57
1:A:120:THR:HG23	1:A:139:ARG:CZ	2.34	0.57
2:F:153:LYS:NZ	2:F:156:ASN:CG	2.56	0.57
3:D:9:VAL:HG12	3:D:115:THR:HB	1.85	0.57
2:C:63:PRO:HB2	2:C:65:ARG:HD3	1.87	0.56
1:B:52:PHE:HB2	1:B:108:MET:HB2	1.87	0.56
1:B:94:ARG:NH2	1:B:117:ASP:OD2	2.37	0.56
3:G:23:LYS:NZ	3:G:77:THR:OG1	2.38	0.56
2:F:124:PRO:HB2	2:F:129:LEU:HD11	1.87	0.56
2:C:150:VAL:HG12	2:C:200:VAL:HG12	1.88	0.56
3:D:130:PRO:HB3	3:D:218:VAL:HG12	1.88	0.56
2:C:136:VAL:HG13	2:C:183:LEU:HB3	1.89	0.55
2:C:117:PRO:HD3	2:C:202:HIS:HD2	1.72	0.55
3:G:2:VAL:HB	3:G:109:TYR:CE1	2.41	0.55
3:D:108:ASP:N	3:D:108:ASP:OD1	2.39	0.55
2:F:153:LYS:HE2	2:F:156:ASN:CA	2.35	0.55
2:C:134:ALA:N	2:C:185:LEU:O	2.39	0.55
3:G:140:GLU:OE1	3:G:141:SER:N	2.40	0.54
2:F:146:ARG:HB2	2:F:177:TYR:CE1	2.43	0.54
3:D:23:LYS:HD2	3:D:78:THR:HG22	1.89	0.54
2:C:13:LEU:HD21	2:C:19:ALA:HB2	1.89	0.54
2:F:125:SER:O	2:F:128:GLN:N	2.39	0.54
2:C:80:SER:OG	2:C:81:SER:N	2.41	0.54
2:C:202:HIS:ND1	2:C:203:GLN:OE1	2.41	0.53
2:F:153:LYS:CE	2:F:156:ASN:CA	2.75	0.53
2:C:142:ASN:HA	2:C:176:THR:HB	1.90	0.53
2:F:153:LYS:HZ1	2:F:156:ASN:CG	2.02	0.53
2:F:205:LEU:HD13	2:F:209:VAL:HG23	1.89	0.53
1:A:35:PRO:O	1:A:137:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:ARG:HE	3:D:109:TYR:HD1	1.56	0.53
3:G:108:ASP:C	3:G:109:TYR:HD2	2.11	0.53
1:A:115:ARG:O	1:A:118:SER:OG	2.27	0.53
2:C:125:SER:HB2	3:D:130:PRO:HG2	1.91	0.53
2:C:199:GLU:OE2	2:C:209:VAL:N	2.42	0.53
2:C:95:SER:HA	2:C:100:LEU:HD22	1.90	0.52
2:F:29:VAL:HA	2:F:96:ARG:HD3	1.90	0.52
2:F:65:ARG:NH2	2:F:86:ASP:OD2	2.42	0.52
1:A:69:ARG:NH2	1:A:118:SER:O	2.43	0.52
2:C:162:ASN:OD1	2:C:184:THR:N	2.31	0.52
2:F:112:ARG:NH1	2:F:115:ALA:HB2	2.24	0.52
2:F:142:ASN:HA	2:F:176:THR:HG23	1.91	0.52
3:G:40:ALA:HB3	3:G:43:GLN:HG3	1.91	0.52
2:C:13:LEU:CD2	2:C:19:ALA:HB2	2.40	0.51
2:C:147:GLU:O	2:C:203:GLN:NE2	2.40	0.51
2:F:41:GLN:HB2	2:F:51:LEU:HD11	1.93	0.51
2:C:154:VAL:HB	2:C:159:GLN:HE21	1.76	0.51
2:C:127:GLU:OE2	2:C:127:GLU:N	2.45	0.50
2:C:140:LEU:HD11	2:C:150:VAL:HG11	1.94	0.50
1:A:90:GLY:HA3	3:G:57:GLY:HA3	1.93	0.50
2:C:14:SER:O	2:C:16:GLY:N	2.45	0.50
2:F:28:GLY:HA2	2:F:73:THR:OG1	2.12	0.50
2:C:12:SER:HB3	2:C:111:LYS:HD3	1.94	0.49
2:C:119:VAL:HG21	2:C:200:VAL:HG21	1.94	0.49
2:F:190:TYR:O	2:F:196:TYR:OH	2.30	0.49
3:G:145:LEU:HD13	3:G:218:VAL:HG21	1.93	0.49
3:G:191:VAL:HG11	3:G:201:TYR:CE2	2.47	0.49
2:F:110:ILE:HB	2:F:175:SER:OG	2.13	0.49
1:B:94:ARG:HB2	1:B:111:VAL:HG12	1.94	0.49
2:F:5:THR:O	2:F:24:ARG:HB3	2.12	0.49
2:C:65:ARG:HH11	2:C:86:ASP:CG	2.15	0.49
1:A:86:ARG:NH2	2:F:96:ARG:HH12	2.11	0.48
2:C:162:ASN:ND2	2:C:184:THR:O	2.46	0.48
3:D:39:GLN:HB2	3:D:45:LEU:HD23	1.94	0.48
1:A:43:VAL:HG12	1:A:143:ARG:HB2	1.95	0.48
1:A:87:SER:OG	3:G:99:ARG:NH1	2.46	0.48
1:A:136:GLU:N	1:A:136:GLU:OE1	2.46	0.48
1:B:51:THR:HA	1:B:109:SER:HA	1.95	0.48
2:C:146:ARG:CZ	2:C:167:VAL:HG11	2.44	0.48
2:F:7:SER:HA	2:F:8:PRO:HA	1.45	0.48
2:F:35:SER:HB2	2:F:55:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:126:PRO:HB3	3:G:152:TYR:HB3	1.95	0.47
1:B:92:ASP:HB3	1:B:95:PHE:HD2	1.79	0.47
2:F:83:GLU:HB3	2:F:85:GLU:OE1	2.15	0.47
2:C:196:TYR:HE1	2:C:215:ARG:HD2	1.79	0.47
2:C:162:ASN:O	2:C:183:LEU:HD12	2.14	0.47
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.47	0.47
1:A:37:PHE:HE1	1:A:108:MET:HG3	1.79	0.47
2:C:63:PRO:HG2	2:C:65:ARG:HH21	1.78	0.47
3:D:172:THR:HG23	3:D:187:SER:HB2	1.97	0.47
2:F:109:GLU:HG3	2:F:170:GLN:OE1	2.15	0.47
1:A:86:ARG:HG3	2:F:96:ARG:O	2.15	0.47
2:F:43:LYS:HG2	2:F:88:ALA:HB2	1.97	0.47
3:D:29:PHE:CE2	3:D:53:PRO:HB3	2.50	0.47
2:F:24:ARG:HH21	2:F:73:THR:HG22	1.81	0.46
1:A:71:SER:HB3	1:A:75:GLN:HB3	1.96	0.46
2:C:196:TYR:CE1	2:C:215:ARG:HD2	2.51	0.46
3:D:172:THR:HA	3:D:187:SER:HA	1.97	0.46
2:C:134:ALA:O	2:C:185:LEU:N	2.42	0.46
3:D:1:GLN:OE1	3:D:1:GLN:N	2.33	0.46
2:C:130:LYS:O	2:C:132:GLY:N	2.45	0.46
3:D:65:LYS:O	3:D:66:ASN:HB2	2.15	0.46
2:F:155:ASP:HB2	2:F:193:HIS:CD2	2.47	0.46
1:A:51:THR:HA	1:A:108:MET:O	2.15	0.45
2:C:1:GLU:HG3	2:C:2:ILE:N	2.31	0.45
2:F:72:GLY:O	2:F:73:THR:OG1	2.29	0.45
2:C:41:GLN:HG3	2:C:90:TYR:CE2	2.51	0.45
2:C:123:PRO:HG3	2:C:213:PHE:CD2	2.52	0.45
1:B:94:ARG:HH22	1:B:114:ARG:CB	2.29	0.45
1:B:35:PRO:HG2	1:B:137:SER:HB3	1.97	0.45
2:F:6:GLN:OE1	2:F:92:CYS:N	2.46	0.45
2:C:154:VAL:HG22	2:C:196:TYR:CD2	2.44	0.45
2:C:87:PHE:HD2	2:C:108:VAL:HG12	1.81	0.45
1:A:120:THR:HG23	1:A:139:ARG:NH2	2.32	0.45
2:C:67:SER:HB2	2:C:78:THR:HG22	1.97	0.45
3:D:131:LEU:HD11	3:D:148:LEU:HB2	1.98	0.45
1:B:53:THR:HA	1:B:106:PHE:O	2.17	0.45
2:F:154:VAL:HG12	2:F:193:HIS:CD2	2.52	0.45
2:C:126:ASP:HA	2:C:129:LEU:HD23	1.98	0.44
2:F:111:LYS:HG3	2:F:144:TYR:OH	2.16	0.44
3:G:28:THR:HB	3:G:31:ASN:HB2	2.00	0.44
3:G:53:PRO:HA	3:G:72:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:PHE:HA	2:F:108:VAL:HG23	1.99	0.44
2:C:194:LYS:HA	2:C:215:ARG:HD3	2.00	0.44
1:A:45:THR:HA	1:A:145:THR:OG1	2.17	0.44
1:B:35:PRO:HG2	1:B:137:SER:CB	2.48	0.44
2:F:1:GLU:HG3	2:F:2:ILE:N	2.32	0.44
1:B:37:PHE:HA	1:B:54:CYS:HA	2.00	0.43
2:C:146:ARG:HB2	2:C:177:TYR:CE2	2.52	0.43
1:B:38:SER:N	1:B:53:THR:O	2.51	0.43
2:F:36:TYR:O	2:F:94:HIS:HA	2.18	0.43
3:G:36:TRP:CD1	3:G:70:LEU:HD22	2.53	0.43
1:A:70:MET:HB2	1:A:120:THR:HG22	2.01	0.43
1:A:94:ARG:NH2	1:A:117:ASP:OD2	2.50	0.43
1:B:37:PHE:CZ	1:B:52:PHE:HD2	2.37	0.43
3:D:6:GLN:N	3:D:112:GLN:HE22	2.15	0.43
2:F:23:CYS:HB2	2:F:39:TRP:CH2	2.53	0.43
2:F:25:ALA:HB3	2:F:73:THR:CG2	2.49	0.43
2:F:199:GLU:OE1	2:F:210:THR:OG1	2.37	0.43
1:A:97:VAL:HG23	1:A:108:MET:CE	2.49	0.43
2:C:164:GLN:HB3	3:D:176:VAL:HG11	2.00	0.43
3:D:153:PHE:HA	3:D:154:PRO:HA	1.76	0.43
2:F:7:SER:O	2:F:22:SER:HB3	2.19	0.43
2:F:165:GLU:OE1	2:F:179:LEU:HD11	2.19	0.42
3:G:189:VAL:HG12	3:G:191:VAL:HG13	2.00	0.42
2:F:125:SER:O	2:F:129:LEU:HD12	2.20	0.42
3:G:198:THR:OG1	3:G:199:LYS:N	2.51	0.42
2:C:154:VAL:HG13	2:C:196:TYR:CE2	2.55	0.42
3:D:36:TRP:CE2	3:D:81:MET:HB2	2.55	0.42
2:F:93:GLN:HG2	2:F:94:HIS:N	2.33	0.42
1:A:87:SER:O	1:A:89:PRO:HD3	2.20	0.42
3:G:153:PHE:HA	3:G:154:PRO:HA	1.80	0.42
3:D:76:THR:O	3:D:78:THR:HG23	2.19	0.41
1:A:99:GLN:HG3	1:A:106:PHE:CE2	2.55	0.41
1:B:39:PRO:CD	1:B:42:LEU:HD21	2.48	0.41
1:A:118:SER:HB3	1:A:144:VAL:H	1.86	0.41
2:C:70:GLY:HA3	2:C:75:PHE:HA	2.02	0.41
2:C:30:SER:OG	2:C:35:SER:OG	2.26	0.41
3:D:170:VAL:O	3:D:171:HIS:HD2	2.03	0.41
2:F:12:SER:HA	2:F:109:GLU:O	2.20	0.41
2:C:203:GLN:OE1	2:C:203:GLN:N	2.30	0.41
1:B:42:LEU:HG	1:B:52:PHE:CE1	2.55	0.41
1:A:70:MET:HB2	1:A:120:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:NH1	1:A:141:GLU:HG2	2.35	0.41
1:B:43:VAL:O	1:B:44:VAL:HB	2.20	0.41
3:D:177:LEU:HD23	3:D:183:TYR:CE1	2.56	0.41
3:D:6:GLN:H	3:D:112:GLN:NE2	2.18	0.40
3:D:67:ARG:HD2	3:D:84:LYS:O	2.21	0.40
1:A:39:PRO:HG3	1:A:42:LEU:HD13	2.04	0.40
1:B:67:TRP:CD2	1:B:108:MET:HB3	2.56	0.40
2:F:167:VAL:HG22	2:F:179:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	91/114 (80%)	82 (90%)	7 (8%)	2 (2%)	6 24
1	B	93/114 (82%)	79 (85%)	11 (12%)	3 (3%)	4 16
2	C	213/218 (98%)	192 (90%)	14 (7%)	7 (3%)	4 15
2	F	213/218 (98%)	199 (93%)	10 (5%)	4 (2%)	8 28
3	D	191/218 (88%)	182 (95%)	9 (5%)	0	100 100
3	G	216/218 (99%)	208 (96%)	7 (3%)	1 (0%)	29 61
All	All	1017/1100 (92%)	942 (93%)	58 (6%)	17 (2%)	9 31

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ARG
1	B	101	PRO
1	B	116	ASN
1	B	117	ASP

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Mol	Chain	Res	Type
2	C	80	SER
2	C	130	LYS
2	C	155	ASP
2	F	72	GLY
2	C	133	THR
2	F	16	GLY
1	A	71	SER
2	C	16	GLY
2	C	173	LYS
2	F	15	PRO
2	F	73	THR
2	C	15	PRO
3	G	2	VAL

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	75/100 (75%)	69 (92%)	6 (8%)	12 33
1	B	68/100 (68%)	64 (94%)	4 (6%)	19 49
2	C	175/189 (93%)	169 (97%)	6 (3%)	37 71
2	F	187/189 (99%)	183 (98%)	4 (2%)	53 81
3	D	168/188 (89%)	164 (98%)	4 (2%)	49 79
3	G	183/188 (97%)	180 (98%)	3 (2%)	62 86
All	All	856/954 (90%)	829 (97%)	27 (3%)	39 73

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	MET
1	A	74	ASN
1	A	77	ASP
1	A	93	SER
1	A	118	SER

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Mol	Chain	Res	Type
1	A	139	ARG
1	B	41	LEU
1	B	52	PHE
1	B	65	LEU
1	B	85	ASP
2	C	24	ARG
2	C	37	LEU
2	C	65	ARG
2	C	86	ASP
2	C	189	ASP
2	C	198	CYS
3	D	7	SER
3	D	101	TYR
3	D	123	THR
3	D	204	ASN
2	F	81	SER
2	F	95	SER
2	F	173	LYS
2	F	184	THR
3	G	1	GLN
3	G	13	LYS
3	G	179	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	142	ASN
3	D	171	HIS
2	F	46	GLN
2	F	170	GLN
2	F	193	HIS
3	G	39	GLN

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	97/114 (85%)	0.45	3 (3%) 49 44	42, 74, 102, 117	0
1	B	101/114 (88%)	0.82	12 (11%) 4 3	55, 80, 108, 116	0
2	C	215/218 (98%)	0.45	11 (5%) 28 24	41, 78, 96, 104	0
2	F	215/218 (98%)	0.34	7 (3%) 46 41	37, 61, 89, 95	0
3	D	197/218 (90%)	-0.09	4 (2%) 65 63	31, 48, 87, 104	0
3	G	218/218 (100%)	0.03	11 (5%) 28 25	28, 45, 93, 110	0
All	All	1043/1100 (94%)	0.28	48 (4%) 32 29	28, 64, 95, 117	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	72	GLY	6.3
3	D	145	LEU	5.8
2	F	115	ALA	5.1
1	A	103	GLY	5.0
3	G	165	ALA	4.2
1	B	144	VAL	4.1
2	C	210	THR	4.0
1	B	115	ARG	4.0
3	G	198	THR	3.5
3	G	26	GLY	3.4
3	G	195	SER	3.3
1	A	35	PRO	3.3
1	B	43	VAL	3.2
2	F	177	TYR	3.2
2	C	81	SER	3.2
2	F	143	PHE	3.1
1	B	126	ILE	2.9
2	C	160	SER	2.9
2	C	126	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	165	ALA	2.8
2	F	114	VAL	2.8
2	C	209	VAL	2.8
3	G	2	VAL	2.8
3	G	166	LEU	2.8
1	B	134	ILE	2.7
2	C	21	LEU	2.6
1	B	114	ARG	2.5
1	B	56	PHE	2.5
1	B	113	ALA	2.5
1	A	34	PRO	2.5
2	C	148	ALA	2.4
1	B	142	LEU	2.4
3	G	1	GLN	2.4
3	G	137	SER	2.4
3	G	3	GLN	2.3
1	B	93	SER	2.3
2	C	111	LYS	2.3
3	G	196	LEU	2.3
2	C	14	SER	2.3
2	F	92	CYS	2.2
2	C	13	LEU	2.2
3	D	167	THR	2.1
2	F	173	LYS	2.1
3	G	66	ASN	2.1
2	C	131	SER	2.1
3	D	164	GLY	2.1
1	B	47	GLY	2.0
1	B	34	PRO	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.