Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 10:05 AM EDT

PDB ID	:	6AVG
Title	:	Crystal structure of the KFJ37 TCR-NY-ESO-1-HLA-B*07:02 complex
Authors	:	Gully, B.S.; Gras, S.; Rossjohn, J.
Deposited on	:	2017-09-02
Resolution	:	2.60 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:

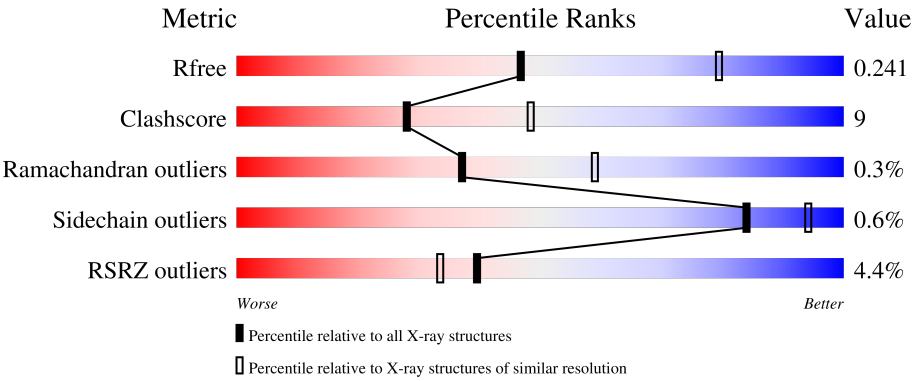
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	107	77% 16% 7%
1	H	107	80% 12% 7%
2	B	202	5% 80% 16%
2	C	202	5% 79% 18%
3	D	245	2% 83% 16%

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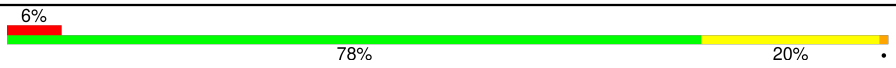
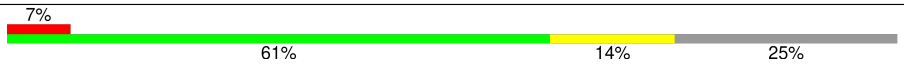
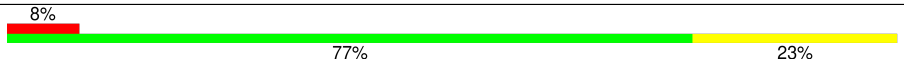
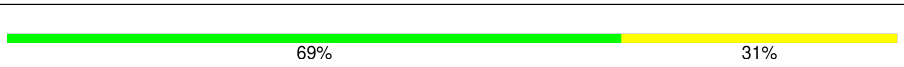
Mol	Chain	Length	Quality of chain
3	E	245	
4	F	362	
4	G	362	
5	P	13	
5	Q	13	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13701 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 Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
1	A	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 2 is a protein called T-cell receptor alpha variable 4,TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	196	Total	C	N	O	S	0	1	0
			1526	958	251	309	8			
2	B	196	Total	C	N	O	S	0	0	0
			1519	955	248	308	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	initiating methionine	UNP A0A0B4J268
C	94	VAL	GLY	conflict	UNP A0A0B4J268
B	3	MET	-	initiating methionine	UNP A0A0B4J268
B	94	VAL	GLY	conflict	UNP A0A0B4J268

- Molecule 3 is a protein called T-cell receptor beta variable 9,TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	245	Total	C	N	O	S	0	0	0
			1933	1216	339	372	6			
3	E	245	Total	C	N	O	S	0	0	0
			1927	1213	336	372	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	MET	-	initiating methionine	UNP A0A0B4J1U6
D	51	GLN	HIS	conflict	UNP A0A0B4J1U6
D	98	GLY	VAL	conflict	UNP A0A0B4J1U6
E	3	MET	-	initiating methionine	UNP A0A0B4J1U6
E	51	GLN	HIS	conflict	UNP A0A0B4J1U6
E	98	GLY	VAL	conflict	UNP A0A0B4J1U6

- Molecule 4 is a protein called HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	272	Total	C	N	O	S	8	0	0
			2221	1381	408	426	6			
4	F	275	Total	C	N	O	S	0	0	0
			2251	1397	413	435	6			

- Molecule 5 is a protein called ALA-PRO-ARG-GLY-PRO-HIS-GLY-GLY-ALA-ALA-SER-GLY-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	13	Total	C	N	O	0	0	0
			81	48	18	15			
5	P	13	Total	C	N	O	0	0	0
			81	48	18	15			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	36	Total	O	0	0
			36	36		
6	C	65	Total	O	0	0
			65	65		
6	D	47	Total	O	0	0
			47	47		
6	G	85	Total	O	0	0
			85	85		
6	A	42	Total	O	0	0
			42	42		
6	B	80	Total	O	0	0
			80	80		
6	E	43	Total	O	0	0
			43	43		
6	F	93	Total	O	0	0
			93	93		

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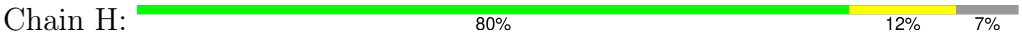
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Q	7	Total O 7 7	0	0
6	P	6	Total O 6 6	0	0

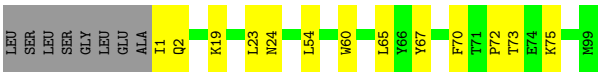
3 Residue-property plots (i)

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: Beta-2-microglobulin

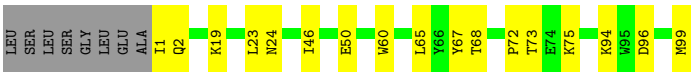
Chain H:





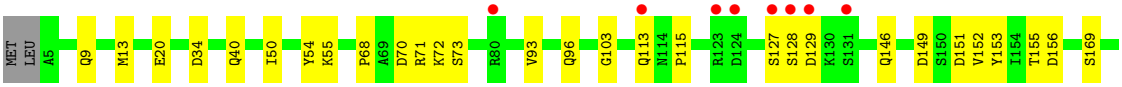
• Molecule 1: Beta-2-microglobulin

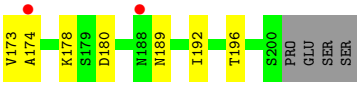
Chain A:



• Molecule 2: T-cell receptor alpha variable 4,TCR alpha chain

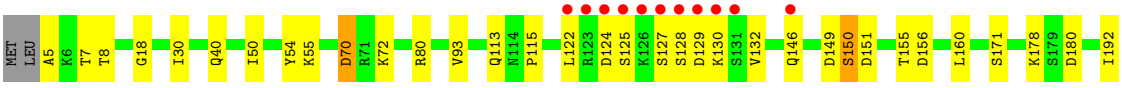
Chain C:

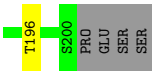




• Molecule 2: T-cell receptor alpha variable 4,TCR alpha chain

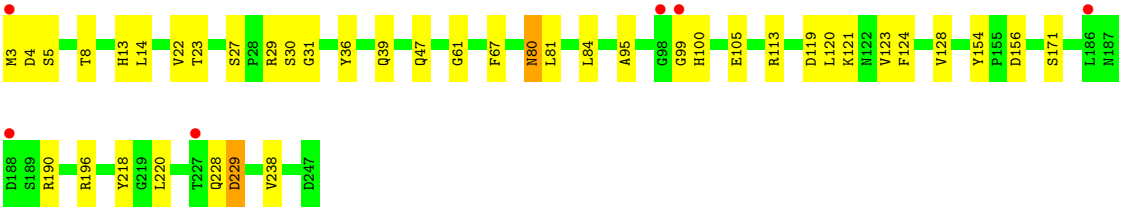
Chain B:



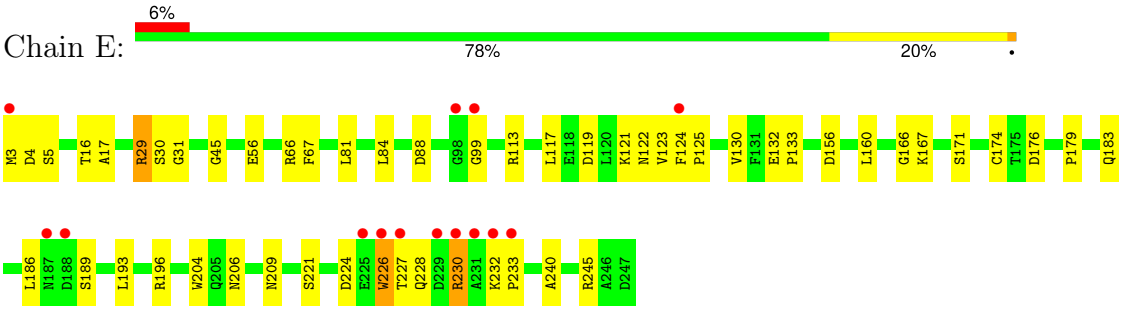


• Molecule 3: T-cell receptor beta variable 9,TCR beta chain

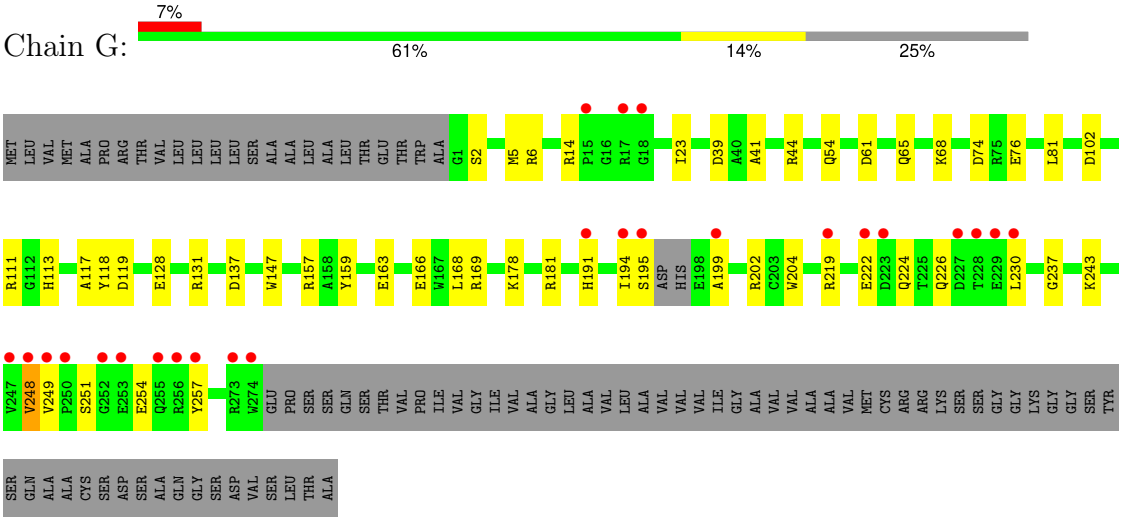
Chain D:



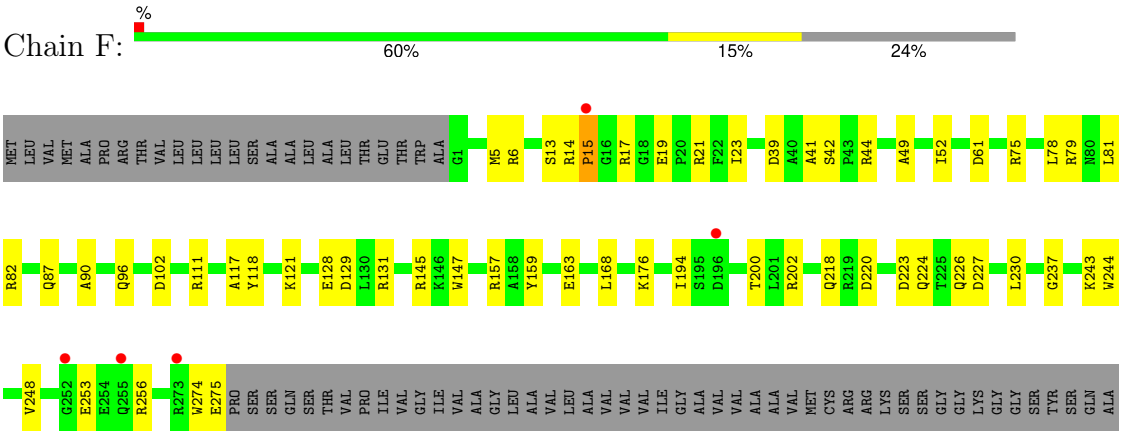
• Molecule 3: T-cell receptor beta variable 9,TCR beta chain



• Molecule 4: HLA class I histocompatibility antigen, B-7 alpha chain



• Molecule 4: HLA class I histocompatibility antigen, B-7 alpha chain



• Molecule 5: ALA-PRO-ARG-GLY-PRO-HIS-GLY-GLY-ALA-ALA-SER-GLY-LEU

Chain Q:

• Molecule 5: ALA-PRO-ARG-GLY-PRO-HIS-GLY-GLY-ALA-ALA-SER-GLY-LEU

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.81Å 74.86Å 96.28Å 94.22° 97.88° 90.16°	Depositor
Resolution (Å)	38.81 – 2.60 38.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.81-2.60) 98.8 (38.81-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.193 , 0.248 0.194 , 0.241	Depositor DCC
R_{free} test set	2875 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.6	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	0.92	EDS
Total number of atoms	13701	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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	0.25	0/852	0.45	0/1152
1	H	0.25	0/852	0.47	0/1152
2	B	0.27	0/1552	0.56	0/2117
2	C	0.26	0/1559	0.50	0/2127
3	D	0.26	0/1984	0.51	0/2699
3	E	0.33	0/1978	0.56	1/2692 (0.0%)
4	F	0.27	0/2313	0.51	1/3142 (0.0%)
4	G	0.29	0/2281	0.57	0/3097
5	P	0.29	0/83	0.87	0/110
5	Q	0.25	0/83	0.81	0/110
All	All	0.28	0/13537	0.53	2/18398 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	226	TRP	CA-CB-CG	-6.90	100.60	113.70
4	F	224	GLN	CA-CB-CG	5.82	126.20	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	829	0	794	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	829	0	794	9	0
2	B	1519	0	1433	24	0
2	C	1526	0	1434	26	0
3	D	1933	0	1826	32	0
3	E	1927	0	1815	41	0
4	F	2251	0	2094	43	0
4	G	2221	0	2074	45	0
5	P	81	0	79	3	0
5	Q	81	0	79	4	0
6	A	42	0	0	4	1
6	B	80	0	0	5	1
6	C	65	0	0	7	0
6	D	47	0	0	5	0
6	E	43	0	0	7	0
6	F	93	0	0	6	0
6	G	85	0	0	11	0
6	H	36	0	0	1	0
6	P	6	0	0	0	0
6	Q	7	0	0	1	0
All	All	13701	0	12422	225	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 9.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:191:HIS:HE1	4:G:199:ALA:HB1	1.26	1.00
3:D:80:ASN:HD22	3:D:80:ASN:N	1.63	0.95
3:E:179:PRO:O	6:E:301:HOH:O	1.84	0.93
1:A:1:ILE:HD11	4:F:121:LYS:NZ	1.88	0.87
2:B:149:ASP:HB3	2:B:151:ASP:OD1	1.75	0.86
4:G:169:ARG:NH1	6:G:404:HOH:O	2.09	0.86
2:C:9:GLN:OE1	6:C:301:HOH:O	1.93	0.85
4:G:199:ALA:N	4:G:249:VAL:O	2.10	0.84
4:G:44:ARG:NH2	4:G:61:ASP:OD1	2.10	0.83
3:E:3:MET:HB3	3:E:4:ASP:HA	1.61	0.82
3:D:23:THR:HG22	3:D:80:ASN:HB3	1.61	0.82
1:A:1:ILE:HD11	4:F:121:LYS:HZ2	1.45	0.81
2:C:20:GLU:OE2	6:C:302:HOH:O	1.98	0.80
3:D:171:SER:OG	6:D:301:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:125:PRO:HD3	3:E:233:PRO:HB3	1.64	0.78
3:D:80:ASN:HD22	3:D:80:ASN:H	1.31	0.78
4:F:14:ARG:HB3	4:F:17:ARG:HB2	1.64	0.78
3:D:113:ARG:NH1	3:D:156:ASP:O	2.17	0.77
4:G:191:HIS:CE1	4:G:199:ALA:HB1	2.16	0.77
3:D:3:MET:HB3	3:D:4:ASP:HA	1.66	0.77
4:F:6:ARG:NH2	4:F:102:ASP:OD1	2.17	0.76
4:G:131:ARG:O	6:G:402:HOH:O	2.03	0.75
4:F:41:ALA:O	6:F:402:HOH:O	2.04	0.75
4:G:44:ARG:O	6:G:403:HOH:O	2.05	0.73
2:C:103:GLY:O	6:C:303:HOH:O	2.06	0.73
3:D:80:ASN:N	3:D:80:ASN:ND2	2.37	0.73
1:A:50:GLU:OE1	6:A:101:HOH:O	2.08	0.72
3:E:3:MET:SD	6:E:337:HOH:O	2.47	0.71
2:C:54:TYR:O	2:C:71:ARG:NH1	2.23	0.70
2:C:155:THR:HG21	3:D:196:ARG:HH12	1.56	0.69
2:B:7:THR:O	6:B:301:HOH:O	2.09	0.69
2:B:40:GLN:HB2	2:B:50:ILE:HD11	1.75	0.69
4:F:176:LYS:NZ	6:F:405:HOH:O	2.25	0.69
2:B:30:ILE:O	6:B:302:HOH:O	2.11	0.68
2:B:70:ASP:HB3	2:B:72:LYS:HG3	1.74	0.68
4:G:74:ASP:OD2	6:G:406:HOH:O	2.11	0.68
2:C:129:ASP:O	6:C:304:HOH:O	2.11	0.67
3:E:160:LEU:O	6:E:302:HOH:O	2.12	0.67
2:C:40:GLN:HB2	2:C:50:ILE:HD11	1.78	0.66
2:B:5:ALA:O	6:B:303:HOH:O	2.12	0.66
3:E:119:ASP:OD2	3:E:121:LYS:HG3	1.96	0.66
3:D:81:LEU:HB3	3:D:84:LEU:HD21	1.78	0.64
3:D:39:GLN:OE1	6:D:302:HOH:O	2.15	0.64
3:D:3:MET:N	3:D:29:ARG:HE	1.94	0.64
1:H:54:LEU:HB3	4:G:23:ILE:HD13	1.79	0.64
4:F:79:ARG:NH2	6:F:407:HOH:O	2.31	0.64
4:G:219:ARG:HB2	4:G:224:GLN:HE21	1.63	0.63
3:E:81:LEU:HB3	3:E:84:LEU:HD21	1.79	0.62
1:A:1:ILE:HD11	4:F:121:LYS:HZ3	1.64	0.62
2:C:113:GLN:C	2:C:115:PRO:HD3	2.19	0.62
4:F:44:ARG:NH2	4:F:61:ASP:OD1	2.29	0.62
4:G:111:ARG:NH2	4:G:128:GLU:OE2	2.33	0.61
2:C:70:ASP:HB2	2:C:72:LYS:HG3	1.83	0.60
3:E:3:MET:HB3	3:E:4:ASP:CA	2.31	0.60
4:F:96:GLN:OE1	6:F:403:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:131:ARG:HH12	4:F:157:ARG:NH2	1.99	0.60
4:F:147:TRP:HE1	5:Q:11:SER:HB2	1.66	0.60
3:E:183:GLN:O	3:E:189:SER:OG	2.11	0.59
4:F:220:ASP:OD2	4:F:256:ARG:NH2	2.31	0.59
4:F:200:THR:HG22	4:F:248:VAL:HG22	1.84	0.59
4:G:5:MET:HB2	4:G:168:LEU:HD13	1.84	0.59
2:C:149:ASP:HB3	2:C:151:ASP:OD1	2.03	0.59
3:E:226:TRP:HE1	3:E:228:GLN:HA	1.68	0.59
4:G:137:ASP:OD1	6:G:407:HOH:O	2.17	0.58
2:C:155:THR:HG21	3:D:196:ARG:NH1	2.18	0.58
4:G:254:GLU:HA	4:G:257:TYR:CD2	2.38	0.58
3:E:167:LYS:NZ	6:E:308:HOH:O	2.37	0.57
4:G:131:ARG:HH12	4:G:157:ARG:NH2	2.02	0.57
4:G:230:LEU:HD11	4:G:243:LYS:HE3	1.85	0.57
4:G:54:GLN:NE2	6:G:414:HOH:O	2.31	0.57
3:E:56:GLU:OE2	4:F:75:ARG:NH2	2.37	0.56
3:E:171:SER:OG	6:E:303:HOH:O	2.18	0.56
3:E:226:TRP:NE1	3:E:228:GLN:HA	2.20	0.56
4:F:194:ILE:HD11	4:F:200:THR:HG23	1.87	0.56
4:G:219:ARG:HB2	4:G:224:GLN:NE2	2.21	0.56
4:G:2:SER:OG	6:G:405:HOH:O	2.09	0.56
2:B:192:ILE:HD11	2:B:196:THR:HG21	1.87	0.56
5:P:12:GLY:O	5:P:13:LEU:HB2	2.07	0.55
4:G:65:GLN:NE2	6:G:423:HOH:O	2.39	0.55
4:G:14:ARG:NH2	4:G:39:ASP:OD2	2.36	0.55
3:E:226:TRP:NE1	3:E:227:THR:O	2.40	0.55
2:C:34:ASP:O	2:C:71:ARG:NH2	2.36	0.54
3:D:120:LEU:HD13	3:D:220:LEU:HD22	1.89	0.54
1:H:24:ASN:HB3	1:H:65:LEU:HD11	1.89	0.54
4:G:147:TRP:HE1	5:P:11:SER:HB2	1.73	0.54
5:Q:3:ARG:NH1	6:Q:101:HOH:O	2.20	0.54
2:B:171:SER:HB3	6:B:324:HOH:O	2.08	0.53
3:E:166:GLY:C	3:E:167:LYS:HD3	2.27	0.53
2:B:54:TYR:CD2	2:B:55:LYS:HG3	2.43	0.53
2:C:54:TYR:CD2	2:C:55:LYS:HG3	2.44	0.53
3:D:61:GLY:O	6:D:303:HOH:O	2.19	0.53
4:G:111:ARG:HE	4:G:113:HIS:CE1	2.26	0.53
3:D:5:SER:OG	3:D:30:SER:OG	2.25	0.53
1:H:60:TRP:CE2	4:G:117:ALA:HB2	2.43	0.53
4:F:13:SER:HB3	4:F:78:LEU:HD13	1.91	0.53
3:E:226:TRP:CD1	3:E:232:LYS:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:82:ARG:NH1	4:F:87:GLN:O	2.36	0.52
2:B:5:ALA:HB3	2:B:93:VAL:HG21	1.91	0.52
3:E:226:TRP:CZ2	3:E:232:LYS:HD2	2.46	0.51
1:A:96:ASP:HB3	1:A:99:MET:HG3	1.90	0.51
1:A:23:LEU:O	1:A:67:TYR:HA	2.11	0.51
1:A:24:ASN:HB3	1:A:65:LEU:HD11	1.92	0.51
3:D:228:GLN:HG2	3:D:229:ASP:N	2.25	0.50
2:B:18:GLY:O	2:B:80:ARG:NH1	2.45	0.50
4:F:111:ARG:NH2	4:F:128:GLU:OE2	2.44	0.50
3:D:80:ASN:H	3:D:80:ASN:ND2	2.02	0.50
4:G:254:GLU:HA	4:G:257:TYR:CE2	2.47	0.50
4:F:253:GLU:HB2	4:F:256:ARG:HD3	1.92	0.50
3:D:3:MET:HB3	3:D:4:ASP:CA	2.38	0.50
3:E:228:GLN:NE2	3:E:230:ARG:O	2.44	0.50
4:F:5:MET:HB2	4:F:168:LEU:HD13	1.93	0.50
1:H:23:LEU:O	1:H:67:TYR:HA	2.12	0.49
4:G:6:ARG:NH1	4:G:102:ASP:OD1	2.43	0.49
4:G:202:ARG:HG2	4:G:204:TRP:NE1	2.28	0.49
3:E:221:SER:N	3:E:224:ASP:OD2	2.41	0.49
5:Q:12:GLY:O	5:Q:13:LEU:HB2	2.13	0.49
2:C:155:THR:HB	2:C:173:VAL:H	1.78	0.49
3:E:132:GLU:OE1	3:E:245:ARG:NH1	2.46	0.48
2:B:155:THR:HG21	3:E:196:ARG:HH12	1.77	0.48
2:C:96:GLN:NE2	6:C:306:HOH:O	2.25	0.48
6:A:103:HOH:O	4:F:237:GLY:HA3	2.13	0.48
2:C:13:MET:HE1	4:F:145:ARG:HG2	1.95	0.48
2:C:192:ILE:HD11	2:C:196:THR:HG21	1.95	0.48
4:G:61:ASP:O	4:G:65:GLN:HG2	2.14	0.48
4:F:147:TRP:NE1	5:Q:11:SER:HB2	2.28	0.47
4:F:21:ARG:HH21	4:F:23:ILE:HD11	1.79	0.47
3:E:122:ASN:OD1	3:E:122:ASN:N	2.46	0.47
3:D:124:PHE:CD1	3:D:190:ARG:HD3	2.50	0.47
4:F:15:PRO:HB3	4:F:90:ALA:O	2.14	0.47
3:D:119:ASP:OD2	3:D:121:LYS:HG3	2.15	0.47
4:F:230:LEU:HD11	4:F:243:LYS:HE3	1.96	0.47
2:C:169:SER:HA	6:C:314:HOH:O	2.15	0.47
4:F:14:ARG:NH2	4:F:21:ARG:HB2	2.29	0.47
4:F:19:GLU:HG3	4:F:75:ARG:NH2	2.30	0.47
3:E:5:SER:OG	3:E:30:SER:OG	2.30	0.47
4:F:14:ARG:NH2	4:F:39:ASP:OD2	2.44	0.47
4:F:42:SER:HA	6:F:402:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:SER:O	2:B:150:SER:OG	2.33	0.46
2:B:155:THR:HG22	2:B:156:ASP:O	2.15	0.46
2:B:130:LYS:HD2	2:B:130:LYS:H	1.80	0.46
3:E:113:ARG:NH2	6:E:314:HOH:O	2.48	0.46
4:F:274:TRP:HA	4:F:275:GLU:HA	1.70	0.46
4:G:131:ARG:HH12	4:G:157:ARG:CZ	2.28	0.46
3:D:47:GLN:OE1	6:D:302:HOH:O	2.21	0.46
1:H:1:ILE:HG13	4:G:119:ASP:O	2.16	0.45
3:D:31:GLY:O	3:D:99:GLY:HA3	2.17	0.45
3:E:113:ARG:NH1	3:E:156:ASP:O	2.50	0.45
1:A:60:TRP:CE2	4:F:117:ALA:HB2	2.51	0.45
3:D:105:GLU:OE1	6:D:304:HOH:O	2.21	0.45
3:D:128:VAL:HG21	3:D:238:VAL:O	2.16	0.45
3:D:67:PHE:CE1	3:D:81:LEU:HG	2.52	0.45
4:G:81:LEU:HD13	4:G:118:TYR:CD1	2.52	0.45
2:B:178:LYS:HD3	2:B:180:ASP:HB3	1.99	0.45
3:E:166:GLY:O	3:E:167:LYS:HD3	2.17	0.45
2:B:146:GLN:H	2:B:146:GLN:CD	2.19	0.45
3:E:130:VAL:HG23	3:E:240:ALA:HB3	1.99	0.45
3:D:22:VAL:HG22	3:D:84:LEU:HD11	1.99	0.44
1:H:73:THR:HG22	1:H:75:LYS:H	1.81	0.44
2:C:153:TYR:O	2:C:174:ALA:HA	2.17	0.44
3:E:17:ALA:HA	3:E:117:LEU:O	2.16	0.44
3:E:176:ASP:HB2	3:E:193:LEU:HD12	2.00	0.44
1:A:46:ILE:O	6:A:102:HOH:O	2.21	0.44
4:F:87:GLN:NE2	6:F:417:HOH:O	2.48	0.44
4:F:81:LEU:HD13	4:F:118:TYR:CD1	2.53	0.44
4:F:218:GLN:HG2	4:F:223:ASP:HA	2.00	0.44
2:B:70:ASP:N	2:B:70:ASP:OD1	2.51	0.44
3:E:31:GLY:O	3:E:99:GLY:HA3	2.18	0.44
3:E:206:ASN:HB3	3:E:209:ASN:ND2	2.32	0.44
1:A:1:ILE:HD12	1:A:1:ILE:O	2.18	0.44
4:F:202:ARG:HD2	4:F:244:TRP:CD2	2.53	0.44
3:D:13:HIS:CD2	3:D:218:TYR:HB3	2.53	0.43
4:G:76:GLU:HB3	6:G:420:HOH:O	2.19	0.43
2:B:124:ASP:HA	2:B:125:SER:HA	1.76	0.43
4:G:68:LYS:O	6:G:408:HOH:O	2.21	0.43
4:G:178:LYS:O	4:G:181:ARG:HB3	2.19	0.43
1:A:23:LEU:HB3	1:A:68:THR:HG22	2.01	0.43
3:E:45:GLY:O	6:E:304:HOH:O	2.21	0.43
2:C:151:ASP:OD1	2:C:152:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:159:TYR:HA	4:F:163:GLU:OE1	2.19	0.43
2:C:155:THR:HG22	2:C:156:ASP:O	2.19	0.43
3:E:122:ASN:HA	3:E:124:PHE:CE2	2.54	0.43
1:A:94:LYS:NZ	6:A:109:HOH:O	2.52	0.42
3:E:3:MET:HG3	3:E:29:ARG:NH1	2.33	0.42
1:A:1:ILE:HA	1:A:2:GLN:HG3	2.01	0.42
3:E:66:ARG:NH1	3:E:88:ASP:OD2	2.39	0.42
3:E:123:VAL:O	3:E:233:PRO:HG3	2.19	0.42
4:F:226:GLN:O	4:F:227:ASP:HB2	2.19	0.42
2:C:68:PRO:HD2	2:C:73:SER:O	2.19	0.42
3:D:36:TYR:HB2	3:D:95:ALA:HB3	2.00	0.42
2:B:8:THR:HA	6:B:349:HOH:O	2.19	0.42
1:H:1:ILE:HA	1:H:2:GLN:HG3	2.00	0.42
4:G:199:ALA:O	4:G:249:VAL:N	2.44	0.42
4:G:254:GLU:HA	4:G:257:TYR:HD2	1.83	0.42
2:B:127:SER:HA	2:B:128:SER:HA	1.79	0.42
3:E:67:PHE:CE1	3:E:81:LEU:HG	2.54	0.42
3:E:226:TRP:CD1	3:E:228:GLN:HA	2.55	0.42
4:F:129:ASP:O	4:F:131:ARG:HG3	2.19	0.42
2:C:146:GLN:O	2:C:189:ASN:ND2	2.50	0.42
4:G:147:TRP:NE1	5:P:11:SER:HB2	2.33	0.42
6:C:361:HOH:O	4:G:166:GLU:HG2	2.19	0.42
1:H:23:LEU:HB2	1:H:70:PHE:CE2	2.55	0.42
4:G:199:ALA:O	4:G:248:VAL:HA	2.20	0.42
3:D:123:VAL:HG23	3:D:154:TYR:O	2.20	0.41
1:A:19:LYS:O	1:A:72:PRO:HD2	2.20	0.41
2:B:160:LEU:HB3	3:E:174:CYS:HB2	2.02	0.41
2:B:113:GLN:C	2:B:115:PRO:HD3	2.40	0.41
4:G:249:VAL:HG11	4:G:257:TYR:CE1	2.56	0.41
3:E:133:PRO:HD2	3:E:204:TRP:CZ2	2.55	0.41
3:D:8:THR:OG1	3:D:27:SER:HB2	2.20	0.41
1:H:19:LYS:O	1:H:72:PRO:HD2	2.20	0.41
4:G:159:TYR:HA	4:G:163:GLU:OE1	2.21	0.41
2:C:127:SER:HA	2:C:128:SER:HA	1.92	0.41
4:G:41:ALA:HB3	6:G:448:HOH:O	2.20	0.41
2:C:178:LYS:HE3	2:C:180:ASP:HB3	2.02	0.41
4:G:194:ILE:H	4:G:195:SER:HA	1.86	0.41
6:H:105:HOH:O	4:G:237:GLY:HA3	2.20	0.41
3:D:14:LEU:HD12	3:D:14:LEU:HA	1.88	0.41
4:G:131:ARG:NH1	4:G:157:ARG:NH2	2.69	0.40
4:F:14:ARG:HD3	4:F:17:ARG:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:131:ARG:NH1	4:F:157:ARG:NH2	2.69	0.40
2:B:122:LEU:HD13	2:B:132:VAL:HG12	2.03	0.40
2:C:34:ASP:HB3	2:C:93:VAL:HB	2.04	0.40
3:D:30:SER:O	3:D:100:HIS:ND1	2.54	0.40
1:A:73:THR:HG22	1:A:75:LYS:H	1.86	0.40
4:F:49:ALA:O	4:F:52:ILE:HG22	2.21	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)
6:A:118:HOH:O	6:B:326:HOH:O[1_565]	2.13	0.07

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	97/107 (91%)	95 (98%)	2 (2%)	0	100	100
1	H	97/107 (91%)	95 (98%)	2 (2%)	0	100	100
2	B	194/202 (96%)	182 (94%)	12 (6%)	0	100	100
2	C	195/202 (96%)	181 (93%)	14 (7%)	0	100	100
3	D	243/245 (99%)	234 (96%)	8 (3%)	1 (0%)	30	52
3	E	243/245 (99%)	231 (95%)	11 (4%)	1 (0%)	30	52
4	F	273/362 (75%)	264 (97%)	8 (3%)	1 (0%)	30	52
4	G	268/362 (74%)	258 (96%)	8 (3%)	2 (1%)	19	38
5	P	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
5	Q	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
All	All	1632/1858 (88%)	1560 (96%)	67 (4%)	5 (0%)	37	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	229	ASP
4	G	226	GLN
4	G	251	SER
3	E	230	ARG
4	F	15	PRO

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	94/100 (94%)	94 (100%)	0	100 100
1	H	94/100 (94%)	94 (100%)	0	100 100
2	B	174/186 (94%)	171 (98%)	3 (2%)	56 78
2	C	174/186 (94%)	174 (100%)	0	100 100
3	D	209/212 (99%)	208 (100%)	1 (0%)	86 95
3	E	208/212 (98%)	205 (99%)	3 (1%)	62 82
4	F	232/297 (78%)	232 (100%)	0	100 100
4	G	228/297 (77%)	226 (99%)	2 (1%)	75 90
5	P	6/6 (100%)	6 (100%)	0	100 100
5	Q	6/6 (100%)	6 (100%)	0	100 100
All	All	1425/1602 (89%)	1416 (99%)	9 (1%)	84 94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	80	ASN
4	G	222	GLU
4	G	248	VAL
2	B	70	ASP
2	B	129	ASP
2	B	150	SER
3	E	16	THR

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Mol	Chain	Res	Type
3	E	29	ARG
3	E	186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	80	ASN
4	G	224	GLN
3	E	183	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 oligosaccharides 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	99/107 (92%)	-0.56	0 100 100	16, 25, 50, 66	0
1	H	99/107 (92%)	-0.49	0 100 100	20, 28, 51, 65	0
2	B	196/202 (97%)	-0.02	11 (5%) 31 25	15, 32, 92, 125	0
2	C	196/202 (97%)	-0.02	10 (5%) 34 29	16, 32, 80, 115	1 (0%)
3	D	245/245 (100%)	0.05	6 (2%) 59 54	17, 43, 73, 90	0
3	E	245/245 (100%)	0.25	14 (5%) 30 25	17, 46, 86, 125	0
4	F	275/362 (75%)	-0.28	5 (1%) 67 62	16, 28, 65, 92	0
4	G	272/362 (75%)	-0.01	25 (9%) 16 13	17, 29, 103, 124	2 (0%)
5	P	13/13 (100%)	-0.02	1 (7%) 21 17	17, 21, 34, 38	0
5	Q	13/13 (100%)	-0.21	0 100 100	14, 20, 35, 35	0
All	All	1653/1858 (88%)	-0.07	72 (4%) 39 33	14, 35, 82, 125	3 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	127	SER	6.0
2	B	125	SER	5.7
2	B	126	LYS	5.5
4	G	18	GLY	5.0
2	B	129	ASP	4.4
3	E	231	ALA	4.4
3	E	226	TRP	4.2
2	B	123	ARG	4.1
4	G	199	ALA	3.8
2	C	128	SER	3.7
2	B	128	SER	3.7
3	E	229	ASP	3.7
3	D	3	MET	3.7

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Mol	Chain	Res	Type	RSRZ
4	G	257	TYR	3.6
4	G	248	VAL	3.6
3	D	99	GLY	3.5
4	G	274	TRP	3.4
4	G	252	GLY	3.3
2	B	131	SER	3.2
3	E	230	ARG	3.2
4	G	249	VAL	3.2
2	B	124	ASP	3.2
4	G	17	ARG	3.1
3	E	98	GLY	3.0
3	E	233	PRO	3.0
3	E	225	GLU	2.9
2	C	80[A]	ARG	2.9
2	C	124	ASP	2.9
4	G	250	PRO	2.9
4	G	195	SER	2.9
4	G	247	VAL	2.8
2	C	113	GLN	2.8
4	F	255	GLN	2.7
5	P	11	SER	2.7
3	E	232	LYS	2.7
2	B	146	GLN	2.7
4	F	15	PRO	2.7
2	C	127	SER	2.7
3	E	99	GLY	2.7
2	B	130	LYS	2.6
3	E	188	ASP	2.6
4	F	273	ARG	2.6
4	G	194	ILE	2.5
4	G	253	GLU	2.5
4	G	255	GLN	2.5
4	G	223	ASP	2.4
4	G	222	GLU	2.4
4	F	252	GLY	2.4
3	E	3	MET	2.4
2	C	174	ALA	2.4
4	G	230	LEU	2.3
4	G	191	HIS	2.3
2	C	123	ARG	2.3
3	D	98	GLY	2.3
3	E	227	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	227	THR	2.2
2	C	188	ASN	2.2
2	B	122	LEU	2.2
4	G	219	ARG	2.2
2	C	129	ASP	2.2
3	E	187	ASN	2.2
4	G	256	ARG	2.1
2	C	131	SER	2.1
4	G	228	THR	2.1
4	G	227	ASP	2.1
3	D	188	ASP	2.1
4	F	196	ASP	2.1
3	E	124	PHE	2.1
4	G	273	ARG	2.1
4	G	15	PRO	2.0
4	G	229	GLU	2.0
3	D	186	LEU	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.