Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:33 am BST

PDB ID	:	5W1V
Title	:	Structure of the HLA-E-VMAPRTLIL/GF4 TCR complex
Authors	:	Gras, S.; Walpole, N.; Farenc, C.; Rossjohn, J.
Deposited on	:	2017-06-04
Resolution	:	3.31 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 following versions of software and data (see references ①) were used in the production of this report:

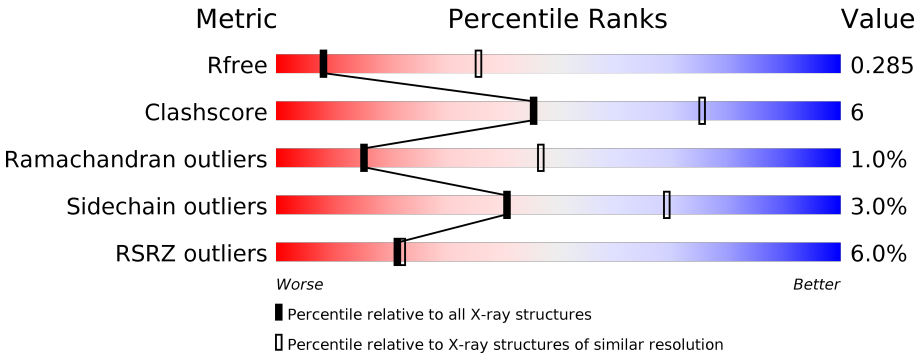
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 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	278	2% 83% 15%
1	F	278	2% 83% 14%
1	K	278	18% 86% 12%
1	P	278	14% 85% 13%
2	B	100	% 79% 21%
2	G	100	% 90% 10%

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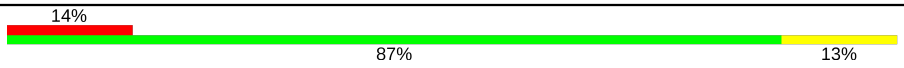
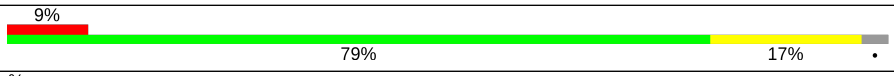
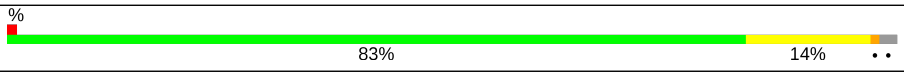
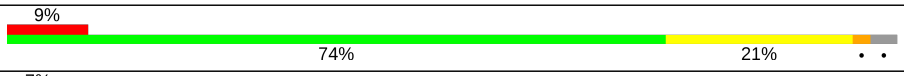
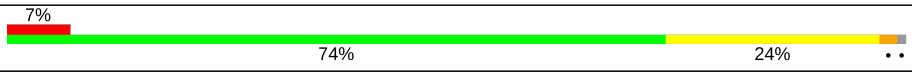
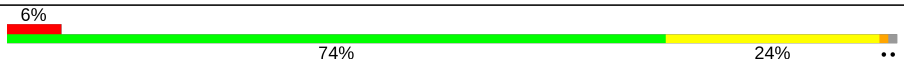
Mol	Chain	Length	Quality of chain
2	L	100	
2	Q	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	207	
4	I	207	
4	N	207	
4	S	207	
5	E	246	
5	J	246	
5	O	246	
5	T	246	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26451 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2221	1392	398	424	7			
1	F	272	Total	C	N	O	S	0	1	0
			2225	1393	396	429	7			
1	K	272	Total	C	N	O	S	0	0	0
			2221	1392	398	424	7			
1	P	272	Total	C	N	O	S	0	1	0
			2230	1397	399	427	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called VMAPRTLIL peptide from CMV gpUL40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			70	46	12	11	1			
3	H	9	Total	C	N	O	S	0	0	0
			70	46	12	11	1			
3	M	9	Total	C	N	O	S	0	0	0
			70	46	12	11	1			
3	R	9	Total	C	N	O	S	0	0	0
			70	46	12	11	1			

- Molecule 4 is a protein called GF4 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1551	975	253	314	9			
4	I	202	Total	C	N	O	S	0	0	0
			1560	980	255	316	9			
4	N	202	Total	C	N	O	S	0	0	0
			1560	980	255	316	9			
4	S	201	Total	C	N	O	S	0	0	0
			1551	975	253	314	9			

- Molecule 5 is a protein called GF4 T cell receptor beta chain.

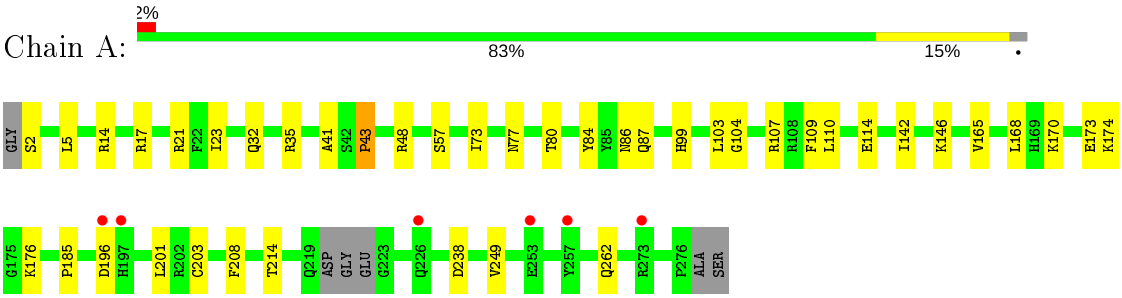
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			
5	J	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			
5	O	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			
5	T	243	Total	C	N	O	S	0	0	0
			1926	1213	334	374	5			

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 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.

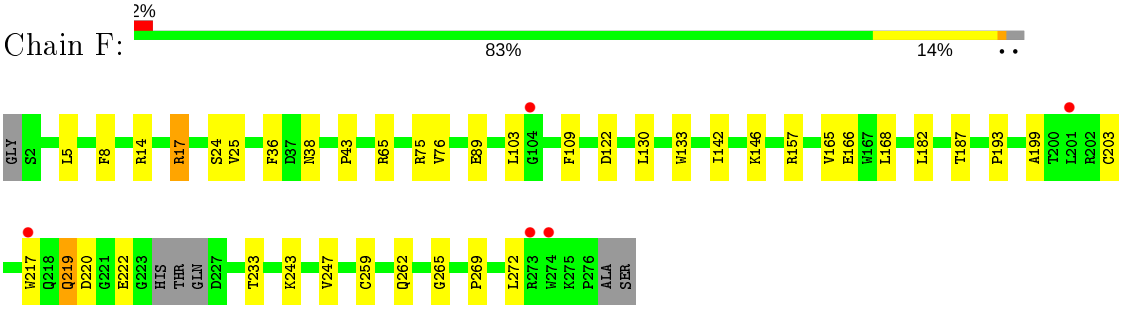
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

Chain A:



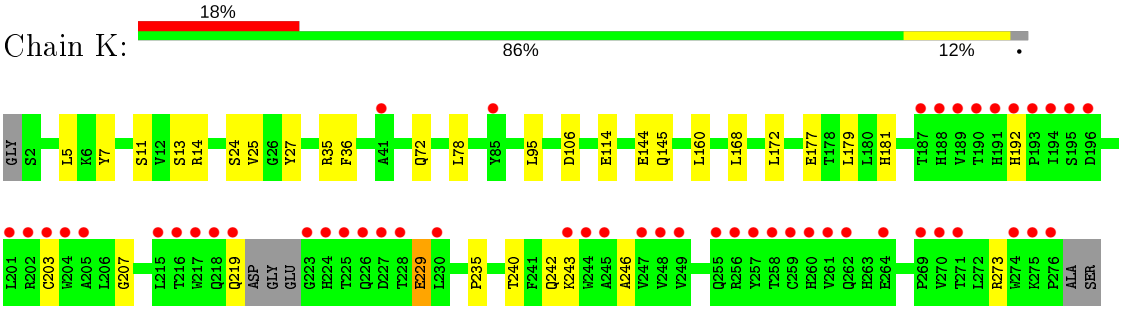
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

Chain F:



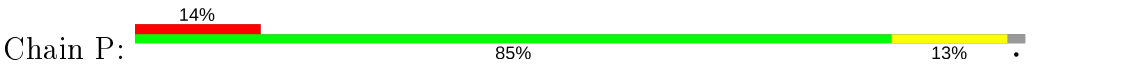
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

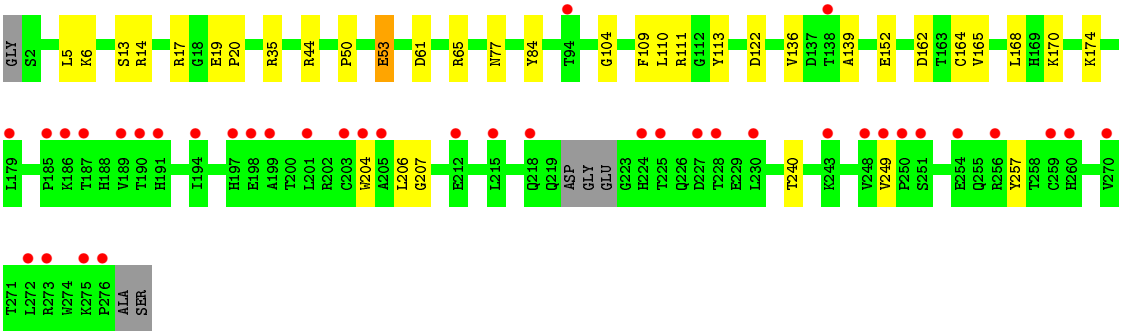
Chain K:



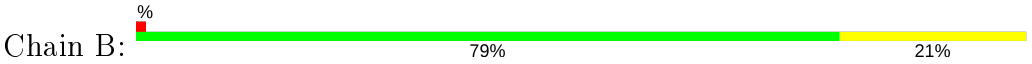
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

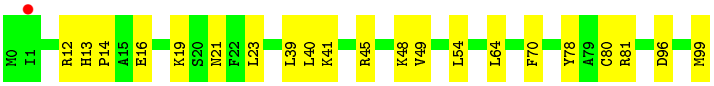
Chain P:



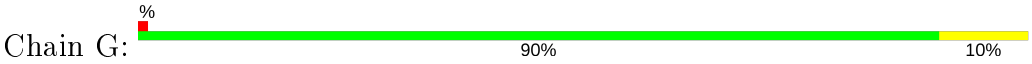


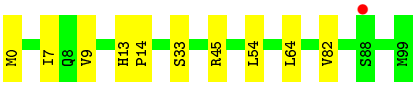
• Molecule 2: Beta-2-microglobulin



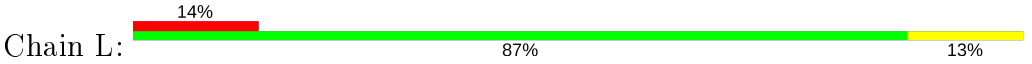


• Molecule 2: Beta-2-microglobulin

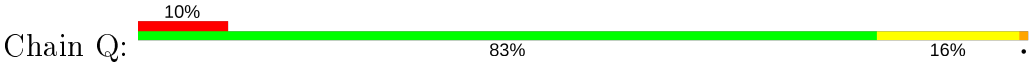


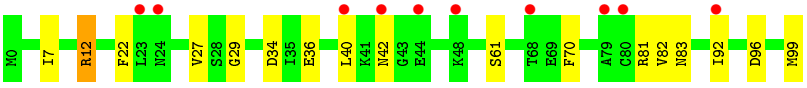


• Molecule 2: Beta-2-microglobulin

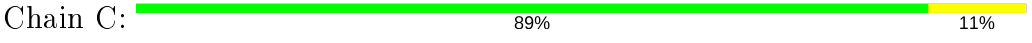


• Molecule 2: Beta-2-microglobulin





• Molecule 3: VMAPRTLIL peptide from CMV gpUL40



• Molecule 3: VMAPRTLIL peptide from CMV gpUL40

Chain H:

• Molecule 3: VMAPRTLIL peptide from CMV gpUL40

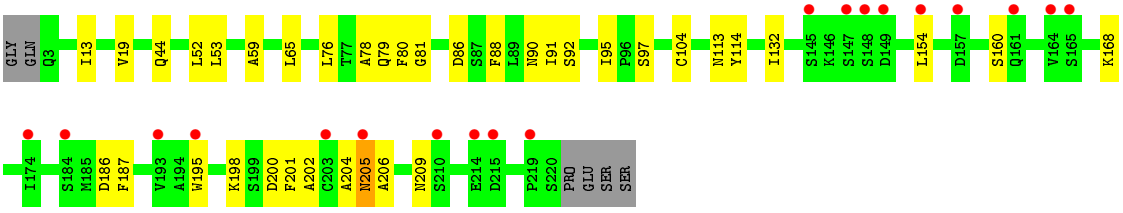
Chain M:

• Molecule 3: VMAPRTLIL peptide from CMV gpUL40

Chain R:

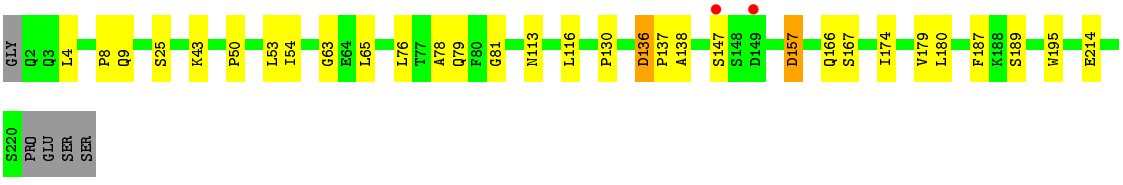
• Molecule 4: GF4 T cell receptor alpha chain

Chain D:



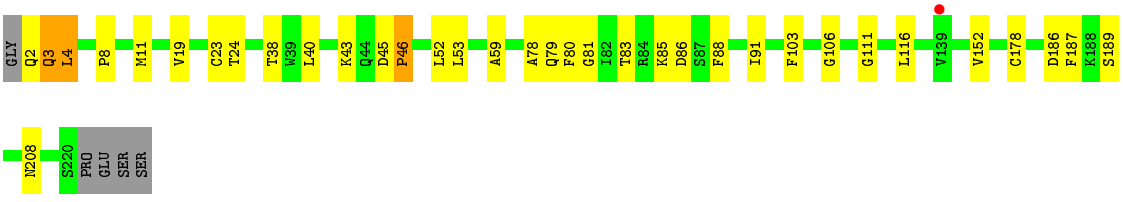
• Molecule 4: GF4 T cell receptor alpha chain

Chain I:



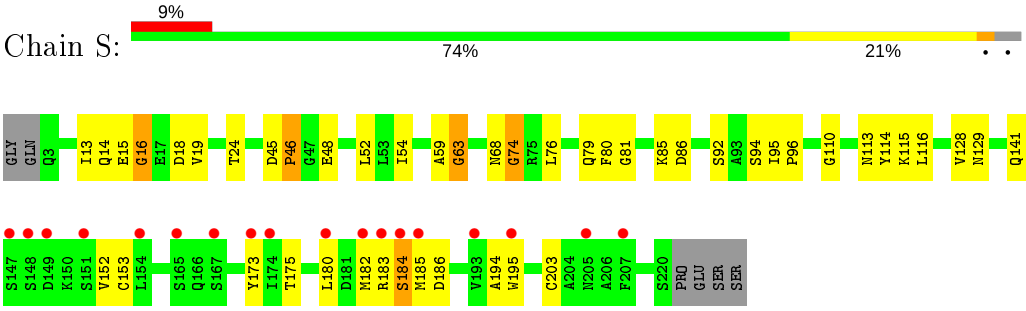
• Molecule 4: GF4 T cell receptor alpha chain

Chain N:



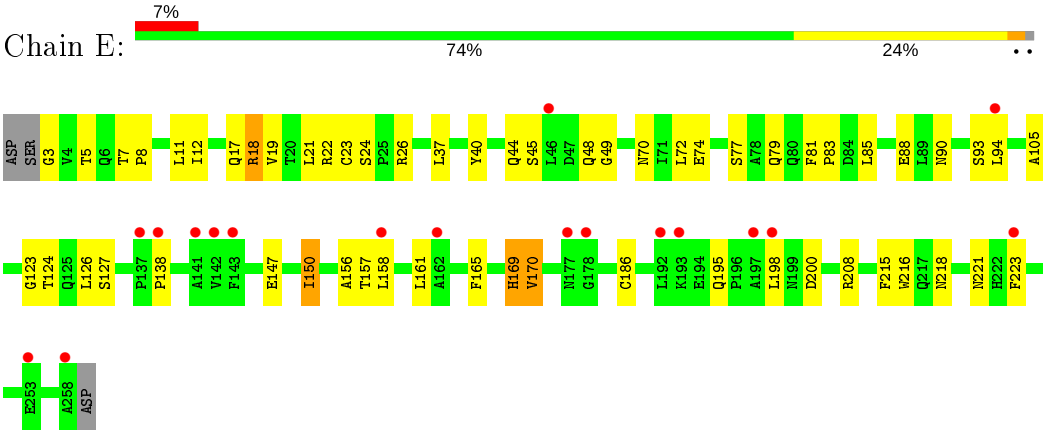
• Molecule 4: GF4 T cell receptor alpha chain

Chain S:



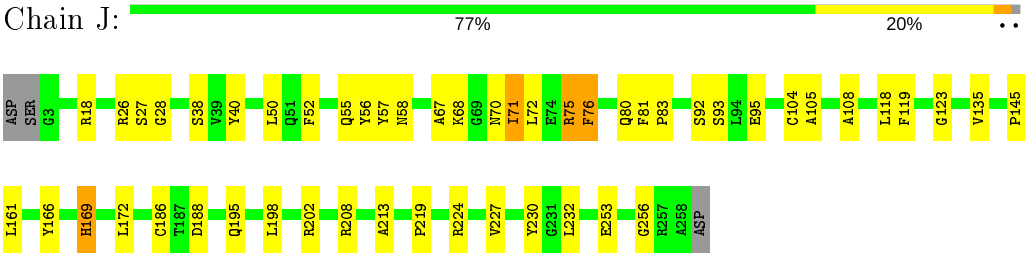
• Molecule 5: GF4 T cell receptor beta chain

Chain E:



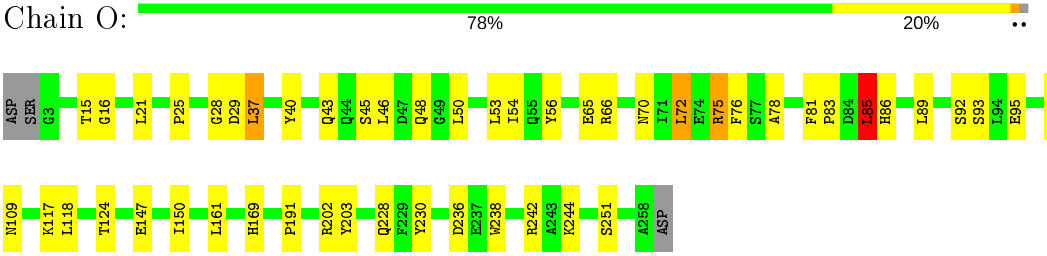
• Molecule 5: GF4 T cell receptor beta chain

Chain J:



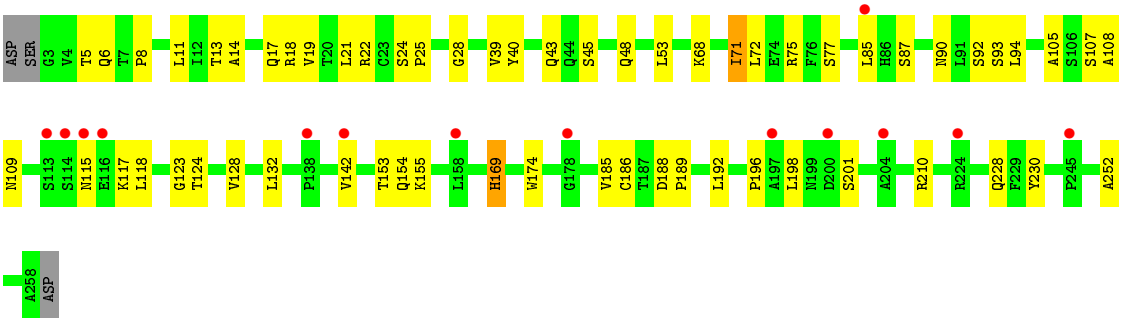
• Molecule 5: GF4 T cell receptor beta chain

Chain O:



• Molecule 5: GF4 T cell receptor beta chain

Chain T:


ASP SER G3 V4 T5 Q6 T7 P8 L11 I12 T13 A14 Q17 R18 V19 T20 L21 R22 C23 S24 P25 G28 V39 Y40 Q43 Q44 S45 Q48 L53 K68 I71 L72 E74 R75 F76 S77 L85 H86 S87 N90 L91 S92 S93 L94 A105 S106 S107 A108
N109 S113 S114 N115 E116 K117 L118 G123 T124 V128 L132 P138 V142 T153 Q154 K155 L158 H169 W174 G178 V185 C186 T187 D188 P189 L192 P196 A197 L198 N199 D200 S201 A204 R210 R224 Q228 F229 Y230 P245 A252
A258 ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.65Å 228.25Å 276.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.93 – 3.31 52.16 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.93-3.31) 99.3 (52.16-3.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.225 , 0.268 0.243 , 0.285	Depositor DCC
R_{free} test set	3445 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	26451	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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	0.39	0/2287	0.47	0/3110
1	F	0.40	0/2290	0.48	0/3113
1	K	0.44	0/2287	0.48	0/3110
1	P	0.39	0/2296	0.45	0/3122
2	B	0.36	0/860	0.49	0/1162
2	G	0.41	0/860	0.47	0/1162
2	L	0.42	0/860	0.48	0/1162
2	Q	0.41	0/860	0.47	0/1162
3	C	0.42	0/70	0.50	0/93
3	H	0.42	0/70	0.48	0/93
3	M	0.48	0/70	0.55	0/93
3	R	0.41	0/70	0.53	0/93
4	D	0.47	0/1585	0.56	0/2151
4	I	0.40	0/1594	0.52	0/2163
4	N	0.43	0/1594	0.53	0/2163
4	S	0.45	0/1585	0.60	2/2151 (0.1%)
5	E	0.40	0/1976	0.51	0/2689
5	J	0.38	0/1976	0.54	0/2689
5	O	0.40	0/1976	0.53	0/2689
5	T	0.41	0/1976	0.53	0/2689
All	All	0.41	0/27142	0.51	2/36859 (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})
4	S	183	ARG	C-N-CA	6.32	137.51	121.70
4	S	185	MET	N-CA-C	-6.28	94.05	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2221	0	2066	20	0
1	F	2225	0	2062	24	0
1	K	2221	0	2066	14	0
1	P	2230	0	2071	20	0
2	B	837	0	803	12	0
2	G	837	0	803	4	0
2	L	837	0	805	9	0
2	Q	837	0	805	8	0
3	C	70	0	85	1	0
3	H	70	0	85	3	0
3	M	70	0	85	2	0
3	R	70	0	85	5	0
4	D	1551	0	1479	25	0
4	I	1560	0	1487	22	0
4	N	1560	0	1489	23	0
4	S	1551	0	1481	31	0
5	E	1926	0	1828	39	0
5	J	1926	0	1828	39	0
5	O	1926	0	1828	36	0
5	T	1926	0	1828	40	0
All	All	26451	0	25069	332	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 6.

All (332) 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:D:204:ALA:O	4:D:206:ALA:N	1.97	0.97
5:J:68:LYS:HE3	5:J:71:ILE:HG13	1.47	0.93
5:J:75:ARG:NH1	5:J:93:SER:O	2.04	0.91
4:N:4:LEU:HD13	4:N:23:CYS:SG	2.21	0.81
3:M:5:ARG:HG3	4:N:111:GLY:O	1.81	0.80
5:O:40:TYR:HB2	5:O:105:ALA:HB3	1.70	0.74
1:F:75:ARG:NH1	5:J:58:ASN:OD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:72:LEU:CD2	5:O:75:ARG:HE	2.01	0.72
5:O:25:PRO:HG2	5:O:85:LEU:HB2	1.69	0.72
2:Q:7:ILE:HG12	2:Q:82:VAL:HG21	1.70	0.71
5:E:45:SER:HB2	5:E:48:GLN:HB3	1.73	0.71
1:P:207:GLY:HA2	1:P:240:THR:HB	1.74	0.70
5:J:81:PHE:HB3	5:J:83:PRO:HD2	1.73	0.69
5:T:21:LEU:HD22	5:T:124:THR:HG21	1.74	0.69
4:I:136:ASP:O	4:I:157:ASP:HB3	1.92	0.69
5:T:45:SER:HB2	5:T:48:GLN:HB2	1.74	0.68
1:F:203:CYS:HB2	1:F:217:TRP:CZ2	2.28	0.68
5:J:40:TYR:HB2	5:J:105:ALA:HB3	1.76	0.67
1:P:6:LYS:HE2	1:P:113:TYR:OH	1.95	0.66
1:F:76:VAL:CG1	5:J:58:ASN:OD1	2.42	0.66
5:J:52:PHE:HZ	5:J:55:GLN:HB2	1.60	0.66
5:T:18:ARG:HH21	5:T:90:ASN:ND2	1.93	0.66
5:T:40:TYR:HB2	5:T:105:ALA:HB3	1.79	0.64
5:O:72:LEU:HB3	5:O:75:ARG:CG	2.28	0.64
5:O:72:LEU:HD23	5:O:75:ARG:HE	1.61	0.64
5:O:105:ALA:HB1	5:O:118:LEU:HD13	1.80	0.64
1:F:24:SER:HB2	1:F:36:PHE:HB3	1.80	0.64
4:N:8:PRO:HG2	4:N:11:MET:SD	2.39	0.63
5:O:75:ARG:NH1	5:O:93:SER:O	2.31	0.63
5:E:17:GLN:HG2	5:E:18:ARG:H	1.64	0.63
5:T:188:ASP:OD1	5:T:189:PRO:HD2	1.99	0.63
4:S:52:LEU:HD23	5:T:117:LYS:HE3	1.81	0.62
5:O:16:GLY:HA2	5:O:93:SER:HB2	1.82	0.62
1:A:41:ALA:O	1:A:43:PRO:HD3	2.00	0.62
5:J:169:HIS:HB3	5:J:230:TYR:HB2	1.81	0.62
4:D:79:GLN:OE1	4:I:81:GLY:HA2	2.01	0.61
5:E:21:LEU:HD22	5:E:124:THR:HG21	1.82	0.61
2:G:33:SER:HB2	2:G:54:LEU:HD11	1.83	0.61
1:P:5:LEU:HB2	1:P:168:LEU:HD13	1.82	0.61
4:N:4:LEU:CD1	4:N:23:CYS:SG	2.89	0.60
4:S:18:ASP:HB3	4:S:92:SER:O	2.01	0.60
5:J:68:LYS:HE3	5:J:71:ILE:CG1	2.27	0.60
5:T:5:THR:HB	5:T:24:SER:HB3	1.82	0.60
5:E:8:PRO:HG3	5:E:11:LEU:HD12	1.84	0.60
5:E:12:ILE:HG22	5:E:127:SER:HB2	1.84	0.60
4:S:141:GLN:HB2	4:S:203:CYS:SG	2.43	0.59
1:A:80:THR:HG22	1:A:84:TYR:HE1	1.67	0.59
1:A:84:TYR:HE2	1:A:142:ILE:HB	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:15:THR:HG23	5:O:95:GLU:HA	1.86	0.58
4:D:76:LEU:HD23	4:D:91:ILE:HG12	1.85	0.58
3:R:8:ILE:HD11	4:S:113:ASN:HD22	1.68	0.58
5:J:76:PHE:HD1	5:J:76:PHE:N	2.01	0.58
5:T:174:TRP:HD1	5:T:185:VAL:HG13	1.69	0.58
1:K:5:LEU:HB2	1:K:168:LEU:HD13	1.84	0.58
5:E:19:VAL:HG23	5:E:94:LEU:HD11	1.86	0.57
1:K:207:GLY:HA2	1:K:240:THR:HB	1.86	0.57
5:E:147:GLU:HA	5:E:150:ILE:HD12	1.86	0.57
4:N:43:LYS:HB2	4:N:53:LEU:HD11	1.86	0.57
5:E:195:GLN:HB3	5:E:198:LEU:HD13	1.87	0.57
1:P:6:LYS:HG2	1:P:113:TYR:OH	2.05	0.57
4:S:182:MET:HE1	5:T:155:LYS:HD3	1.87	0.57
4:S:95:ILE:HG13	4:S:96:PRO:HD2	1.88	0.56
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.87	0.56
4:N:2:GLN:O	4:N:2:GLN:HG3	2.04	0.56
5:T:8:PRO:HG2	5:T:11:LEU:HD13	1.87	0.56
1:A:103:LEU:HD21	1:A:165:VAL:HG13	1.86	0.56
3:C:8:ILE:HD11	4:D:113:ASN:HB3	1.87	0.56
1:P:44:ARG:HH22	1:P:61:ASP:HA	1.71	0.56
2:Q:36:GLU:HB3	2:Q:83:ASN:HB3	1.88	0.56
4:S:13:ILE:HD11	4:S:128:VAL:HG22	1.87	0.56
4:N:103:PHE:CZ	5:O:50:LEU:HD13	2.42	0.55
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.88	0.55
4:I:4:LEU:HD23	4:I:25:SER:HB2	1.88	0.55
5:J:76:PHE:HD1	5:J:76:PHE:H	1.54	0.55
4:N:79:GLN:OE1	4:S:81:GLY:HA2	2.06	0.55
5:T:77:SER:HB2	5:T:90:ASN:HB2	1.87	0.55
5:J:56:TYR:HB3	5:J:80:GLN:OE1	2.07	0.55
5:T:19:VAL:CG2	5:T:94:LEU:HD11	2.36	0.55
4:D:59:ALA:HA	4:D:80:PHE:CD1	2.42	0.54
5:J:75:ARG:NH2	5:J:95:GLU:HB2	2.22	0.54
5:T:6:GLN:HG3	5:T:22:ARG:O	2.07	0.54
5:J:76:PHE:CD1	5:J:76:PHE:N	2.71	0.54
1:A:170:LYS:O	1:A:174:LYS:HG2	2.08	0.54
4:D:52:LEU:HD13	5:E:117:LYS:HG3	1.89	0.54
3:M:9:LEU:H	3:M:9:LEU:HD12	1.72	0.54
5:E:40:TYR:HB2	5:E:105:ALA:HB3	1.90	0.54
5:J:71:ILE:C	5:J:72:LEU:HD12	2.28	0.54
4:I:43:LYS:HB2	4:I:53:LEU:HD11	1.89	0.54
4:S:115:LYS:O	4:S:116:LEU:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HG2	1:A:23:ILE:HD11	1.91	0.53
4:D:53:LEU:HD23	4:D:76:LEU:HD22	1.89	0.53
4:N:78:ALA:HA	4:N:88:PHE:O	2.08	0.53
2:B:39:LEU:HD13	2:B:49:VAL:HG21	1.90	0.53
1:K:192:HIS:CE1	2:L:98:ASP:HB3	2.43	0.53
2:L:30:PHE:HZ	2:L:64:LEU:HD13	1.73	0.53
4:S:182:MET:HE1	5:T:155:LYS:CD	2.38	0.53
1:F:76:VAL:HG21	5:J:57:TYR:OH	2.08	0.53
5:J:172:LEU:HG	5:J:227:VAL:HG22	1.89	0.53
4:N:187:PHE:CZ	4:N:189:SER:HB3	2.44	0.53
5:O:81:PHE:HB3	5:O:83:PRO:CD	2.38	0.53
4:S:182:MET:HG2	4:S:184:SER:HB3	1.90	0.53
1:F:262:GLN:HG2	1:F:269:PRO:HB3	1.91	0.53
5:O:78:ALA:HB2	5:O:89:LEU:HD12	1.90	0.53
5:O:72:LEU:HD22	5:O:75:ARG:HE	1.71	0.53
3:H:8:ILE:HD11	4:I:113:ASN:OD1	2.09	0.52
5:T:25:PRO:HG2	5:T:85:LEU:HD13	1.90	0.52
5:E:7:THR:HB	5:E:22:ARG:HB3	1.91	0.52
1:K:24:SER:HB2	1:K:36:PHE:HB3	1.91	0.52
3:R:4:PRO:HB2	4:S:110:GLY:O	2.09	0.52
5:E:18:ARG:HG2	5:E:19:VAL:N	2.23	0.52
5:J:224:ARG:HG3	5:J:253:GLU:HG2	1.91	0.52
4:S:14:GLN:HG2	4:S:129:ASN:HB3	1.91	0.52
4:S:114:TYR:CE1	5:T:108:ALA:HA	2.45	0.52
4:S:175:THR:HG22	5:T:192:LEU:HD13	1.92	0.52
1:K:114:GLU:HG3	1:K:160:LEU:HD11	1.91	0.51
2:L:54:LEU:CD1	2:L:64:LEU:HD11	2.40	0.51
1:F:217:TRP:CH2	1:F:259:CYS:HB2	2.45	0.51
5:O:28:GLY:O	5:O:37:LEU:HD23	2.10	0.51
5:T:28:GLY:O	5:T:109:ASN:HA	2.10	0.51
2:G:54:LEU:HG	2:G:64:LEU:HD11	1.92	0.51
2:L:54:LEU:HD11	2:L:62:PHE:CD1	2.46	0.51
5:O:72:LEU:O	5:O:75:ARG:HG2	2.11	0.51
5:O:169:HIS:HB3	5:O:230:TYR:HB2	1.93	0.51
4:S:153:CYS:HB2	4:S:194:ALA:HB3	1.92	0.50
4:S:182:MET:O	4:S:186:ASP:HA	2.10	0.50
4:D:168:LYS:HD2	4:D:209:ASN:HB2	1.92	0.50
4:S:152:VAL:HG12	4:S:195:TRP:HB3	1.94	0.50
5:T:39:VAL:HG11	5:T:87:SER:OG	2.10	0.50
1:F:109:PHE:HB2	1:F:165:VAL:HG21	1.94	0.50
5:O:76:PHE:N	5:O:76:PHE:CD1	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:LYS:O	4:D:201:PHE:HB3	2.12	0.50
5:E:169:HIS:HB3	5:E:230:TYR:HB2	1.93	0.50
4:N:152:VAL:HG11	5:O:161:LEU:HD11	1.92	0.50
5:T:45:SER:CB	5:T:48:GLN:HB2	2.39	0.50
5:E:12:ILE:HG23	5:E:169:HIS:HE1	1.76	0.50
1:A:214:THR:HB	1:A:262:GLN:HB2	1.93	0.50
4:D:52:LEU:HD22	5:E:117:LYS:HE3	1.94	0.50
1:P:13:SER:HA	1:P:20:PRO:HB3	1.94	0.49
5:E:81:PHE:HB3	5:E:83:PRO:CD	2.42	0.49
5:J:18:ARG:HA	5:J:92:SER:HB2	1.94	0.49
5:J:195:GLN:HB3	5:J:198:LEU:HD13	1.95	0.49
3:R:8:ILE:HD11	4:S:113:ASN:ND2	2.25	0.49
5:T:6:GLN:OE1	5:T:123:GLY:HA2	2.12	0.49
2:G:13:HIS:HB3	2:G:14:PRO:HD2	1.94	0.49
5:O:72:LEU:HB3	5:O:75:ARG:HG3	1.94	0.49
5:J:18:ARG:HG3	5:J:92:SER:HB2	1.94	0.49
1:P:204:TRP:HE3	1:P:206:LEU:HD21	1.78	0.49
5:O:107:SER:HB3	5:O:118:LEU:HA	1.95	0.48
2:Q:29:GLY:HA2	2:Q:61:SER:HB2	1.95	0.48
4:N:8:PRO:CG	4:N:11:MET:SD	3.01	0.48
1:F:76:VAL:HG12	5:J:58:ASN:OD1	2.13	0.48
1:A:14:ARG:HB3	1:A:17:ARG:HB2	1.94	0.48
4:D:13:ILE:HG13	4:D:19:VAL:HG11	1.95	0.48
5:E:5:THR:OG1	5:E:24:SER:HB3	2.14	0.48
1:F:14:ARG:HB2	1:F:17:ARG:HB2	1.95	0.48
1:F:187:THR:HB	1:F:272:LEU:HD22	1.95	0.48
4:D:198:LYS:HD3	4:D:200:ASP:HB3	1.94	0.48
5:J:219:PRO:HA	5:J:256:GLY:O	2.12	0.48
5:E:77:SER:HB3	5:E:90:ASN:HB2	1.95	0.48
4:I:136:ASP:O	4:I:157:ASP:CB	2.62	0.48
2:B:23:LEU:HD23	2:B:39:LEU:HD23	1.95	0.47
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.96	0.47
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.95	0.47
2:G:7:ILE:HG12	2:G:82:VAL:HG21	1.96	0.47
4:D:154:LEU:HD21	5:E:157:THR:HG21	1.95	0.47
1:F:8:PHE:HB2	1:F:25:VAL:CG2	2.45	0.47
4:I:130:PRO:HG2	4:I:179:VAL:HG21	1.94	0.47
5:J:75:ARG:HH22	5:J:95:GLU:HB2	1.78	0.47
4:N:80:PHE:O	4:N:86:ASP:O	2.33	0.47
5:J:27:SER:HA	5:J:28:GLY:HA2	1.67	0.47
5:O:37:LEU:HG	5:O:108:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LEU:HB2	1:F:168:LEU:HD13	1.96	0.47
1:P:109:PHE:HB2	1:P:165:VAL:HG21	1.97	0.47
5:J:38:SER:HA	5:J:56:TYR:O	2.15	0.47
2:L:54:LEU:HD13	2:L:64:LEU:HD11	1.97	0.47
5:O:21:LEU:HD22	5:O:124:THR:HG21	1.96	0.47
5:T:14:ALA:HB2	5:T:132:LEU:HD11	1.96	0.47
4:D:78:ALA:HA	4:D:88:PHE:O	2.15	0.47
1:P:77:ASN:HB3	3:R:9:LEU:HD12	1.96	0.46
4:N:81:GLY:HA2	4:S:79:GLN:OE1	2.15	0.46
5:T:169:HIS:HB3	5:T:230:TYR:HB2	1.97	0.46
1:A:104:GLY:HA2	1:A:110:LEU:HD12	1.97	0.46
2:L:7:ILE:HG12	2:L:82:VAL:HG21	1.97	0.46
5:O:45:SER:HB3	5:O:48:GLN:HB2	1.97	0.46
5:T:153:THR:O	5:T:154:GLN:HB2	2.15	0.46
1:A:173:GLU:HG2	1:A:176:LYS:HE3	1.97	0.46
1:F:65:ARG:HH22	5:J:67:ALA:HA	1.80	0.46
5:E:169:HIS:O	5:E:170:VAL:HG13	2.16	0.46
5:J:150:ILE:HG23	5:J:213:ALA:HB1	1.96	0.46
1:K:72:GLN:OE1	5:O:66:ARG:HD2	2.16	0.46
4:D:154:LEU:CD2	5:E:157:THR:HG21	2.46	0.46
4:S:182:MET:HE2	4:S:184:SER:OG	2.15	0.46
1:A:35:ARG:HE	1:A:48:ARG:HH11	1.63	0.46
4:I:8:PRO:O	4:I:9:GLN:HB3	2.16	0.46
1:P:50:PRO:HA	1:P:53:GLU:HG2	1.98	0.46
4:S:173:TYR:O	4:S:194:ALA:HA	2.16	0.46
5:T:72:LEU:C	5:T:75:ARG:H	2.19	0.46
5:E:37:LEU:HD23	5:E:85:LEU:HD11	1.97	0.45
4:D:95:ILE:HG23	4:D:97:SER:HB3	1.98	0.45
5:O:147:GLU:HA	5:O:150:ILE:HD12	1.99	0.45
1:F:38:ASN:HA	1:F:43:PRO:HB3	1.98	0.45
1:P:111:ARG:NH2	1:P:113:TYR:HB3	2.32	0.45
5:T:13:THR:HG22	5:T:14:ALA:N	2.32	0.45
5:O:29:ASP:OD1	5:O:109:ASN:HB2	2.17	0.45
5:E:147:GLU:HA	5:E:150:ILE:CD1	2.47	0.45
2:L:73:THR:HB	2:L:76:ASP:HB2	1.98	0.45
1:P:249:VAL:HG11	1:P:257:TYR:CE2	2.52	0.45
1:K:11:SER:HB3	1:K:95:LEU:HB3	1.98	0.45
5:T:198:LEU:HD22	5:T:201:SER:HB2	1.97	0.45
5:T:68:LYS:HD2	5:T:71:ILE:HD11	1.97	0.45
5:O:191:PRO:HB2	5:O:203:TYR:HB3	1.99	0.45
1:P:14:ARG:HD2	1:P:19:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLU:HB2	2:B:19:LYS:HD2	2.00	0.44
4:N:38:THR:O	4:N:106:GLY:HA2	2.17	0.44
5:O:72:LEU:CB	5:O:75:ARG:HG3	2.47	0.44
5:J:135:VAL:HG11	5:J:232:LEU:HD13	1.99	0.44
1:F:103:LEU:HD12	1:F:103:LEU:O	2.17	0.44
1:F:130:LEU:HB2	1:F:157:ARG:HG3	1.99	0.44
5:T:18:ARG:HG3	5:T:92:SER:HB3	1.98	0.44
1:F:75:ARG:HH12	5:J:58:ASN:CG	2.21	0.44
5:J:145:PRO:HD3	5:J:158:LEU:HG	1.99	0.44
1:K:177:GLU:O	1:K:181:HIS:HB2	2.18	0.44
2:Q:7:ILE:HG13	2:Q:27:VAL:HG12	2.00	0.44
1:F:182:LEU:HD13	1:F:265:GLY:HA2	1.98	0.44
5:O:43:GLN:HB2	5:O:53:LEU:HD11	2.00	0.44
4:S:59:ALA:HA	4:S:80:PHE:CD1	2.53	0.44
5:T:94:LEU:HD13	5:T:128:VAL:HG22	1.99	0.44
1:F:193:PRO:HA	1:F:199:ALA:HA	1.98	0.44
5:T:19:VAL:HG21	5:T:94:LEU:HD11	2.00	0.44
5:E:22:ARG:HG2	5:E:23:CYS:N	2.33	0.44
5:J:40:TYR:CZ	5:J:118:LEU:HD11	2.53	0.44
4:D:195:TRP:CE2	5:E:161:LEU:HD11	2.53	0.43
1:F:142:ILE:O	1:F:146:LYS:HB2	2.18	0.43
1:K:229:GLU:HB3	1:K:246:ALA:HB3	2.00	0.43
2:Q:40:LEU:HD11	2:Q:81:ARG:HG3	1.99	0.43
4:I:50:PRO:HG2	5:J:50:LEU:HD11	1.99	0.43
1:P:104:GLY:HA2	1:P:110:LEU:HD12	2.01	0.43
1:P:84:TYR:HB3	1:P:139:ALA:HB1	2.01	0.43
2:B:40:LEU:HD23	2:B:45:ARG:HA	2.00	0.43
5:E:218:ASN:HD22	5:E:221:ASN:ND2	2.16	0.43
5:E:12:ILE:HD11	5:E:231:GLY:C	2.39	0.43
5:J:75:ARG:H	5:J:75:ARG:HG2	1.53	0.43
1:P:122:ASP:HB3	1:P:136:VAL:HG21	2.00	0.43
4:S:54:ILE:HD11	4:S:76:LEU:HB3	2.00	0.43
4:I:167:SER:HB3	4:I:174:ILE:HD12	2.00	0.43
4:I:9:GLN:HG3	4:I:9:GLN:O	2.18	0.43
1:K:13:SER:HB3	1:K:78:LEU:HD13	2.01	0.43
4:S:80:PHE:O	4:S:86:ASP:O	2.37	0.43
1:A:23:ILE:HD13	2:B:54:LEU:HD23	2.00	0.43
5:E:156:ALA:HB2	5:E:216:TRP:CD1	2.53	0.43
1:K:242:GLN:O	1:K:243:LYS:HG3	2.18	0.43
2:B:40:LEU:HD11	2:B:81:ARG:HB2	2.01	0.43
5:E:72:LEU:O	5:E:74:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:52:LEU:HD22	5:O:117:LYS:HE3	2.00	0.43
2:Q:96:ASP:HB3	2:Q:99:MET:HB2	1.99	0.43
5:T:142:VAL:HG23	5:T:252:ALA:HB3	2.00	0.43
1:A:109:PHE:HB2	1:A:165:VAL:HG21	2.01	0.43
2:B:41:LYS:HG3	2:B:78:TYR:CE2	2.54	0.43
4:S:13:ILE:HG12	4:S:19:VAL:HG11	2.00	0.43
5:T:188:ASP:OD1	5:T:189:PRO:CD	2.64	0.43
4:D:80:PHE:O	4:D:86:ASP:O	2.37	0.43
1:F:219:GLN:O	1:F:220:ASP:HB2	2.18	0.43
2:Q:81:ARG:HG2	2:Q:92:ILE:HG12	2.01	0.43
4:D:81:GLY:HA2	4:I:79:GLN:OE1	2.19	0.42
1:P:170:LYS:HB3	1:P:174:LYS:HE2	2.01	0.42
1:F:133:TRP:CH2	3:H:7:LEU:HD11	2.54	0.42
4:D:204:ALA:C	4:D:206:ALA:H	2.02	0.42
4:N:19:VAL:HG13	4:N:91:ILE:HB	2.02	0.42
1:K:7:TYR:HA	1:K:25:VAL:O	2.20	0.42
5:T:155:LYS:HE2	5:T:210:ARG:HH21	1.85	0.42
4:D:19:VAL:O	4:D:90:ASN:HA	2.18	0.42
5:T:18:ARG:HA	5:T:92:SER:HB3	1.99	0.42
2:L:29:GLY:HA2	2:L:61:SER:HB2	2.01	0.42
4:I:116:LEU:CD1	5:J:118:LEU:HD13	2.50	0.42
4:N:3:GLN:HE21	4:N:3:GLN:HA	1.85	0.42
4:N:83:THR:HG23	4:N:85:LYS:H	1.84	0.42
5:O:238:TRP:HB2	5:O:244:LYS:HG3	2.02	0.42
5:O:25:PRO:HG2	5:O:85:LEU:HD22	2.02	0.42
3:H:8:ILE:CD1	4:I:113:ASN:OD1	2.67	0.42
1:A:238:ASP:HB3	2:B:12:ARG:HD3	2.02	0.42
2:B:54:LEU:HD12	2:B:64:LEU:HD11	2.00	0.42
2:B:96:ASP:HB3	2:B:99:MET:HB3	2.01	0.42
5:E:11:LEU:HD22	5:E:126:LEU:HD12	2.01	0.42
5:E:138:PRO:HA	5:E:165:PHE:HB3	2.01	0.42
4:I:53:LEU:HD13	4:I:76:LEU:CD2	2.49	0.42
1:A:142:ILE:O	1:A:146:LYS:HB2	2.20	0.41
4:I:137:PRO:O	4:I:138:ALA:HB2	2.20	0.41
4:I:180:LEU:HB3	5:J:186:CYS:HB2	2.02	0.41
4:I:195:TRP:CD2	5:J:161:LEU:HD21	2.54	0.41
5:O:92:SER:HA	5:O:93:SER:HA	1.82	0.41
5:E:150:ILE:HG12	5:E:216:TRP:HZ2	1.85	0.41
4:D:44:GLN:HE22	5:E:44:GLN:HE22	1.68	0.41
4:I:4:LEU:CD2	4:I:25:SER:HB2	2.48	0.41
1:K:172:LEU:HD23	1:K:179:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:45:ASP:O	4:N:46:PRO:C	2.58	0.41
5:O:56:TYR:CD1	5:O:65:GLU:HA	2.56	0.41
5:E:79:GLN:HE21	5:E:88:GLU:HB2	1.85	0.41
4:I:187:PHE:CZ	4:I:189:SER:HB3	2.55	0.41
4:S:24:THR:HA	4:S:85:LYS:O	2.20	0.41
1:A:73:ILE:HG22	1:A:77:ASN:ND2	2.35	0.41
1:A:99:HIS:HB3	1:A:114:GLU:HG3	2.03	0.41
4:D:114:TYR:HB3	5:E:40:TYR:OH	2.20	0.41
4:N:24:THR:HG22	4:N:86:ASP:OD1	2.20	0.41
4:D:132:ILE:HB	4:D:160:SER:HB2	2.01	0.41
5:E:158:LEU:HD22	5:E:223:PHE:HB3	2.02	0.41
5:T:92:SER:HA	5:T:93:SER:HA	1.81	0.41
4:N:79:GLN:NE2	4:S:63:GLY:HA2	2.35	0.41
1:P:5:LEU:HD23	1:P:164:CYS:SG	2.61	0.41
5:E:3:GLY:HA3	5:E:26:ARG:HG2	2.02	0.41
1:K:14:ARG:O	1:K:14:ARG:HG3	2.21	0.41
1:P:152:GLU:OE2	3:R:5:ARG:NH2	2.53	0.41
5:T:107:SER:HB2	5:T:118:LEU:HD23	2.03	0.41
4:S:68:ASN:O	4:S:74:GLY:C	2.59	0.41
5:T:17:GLN:HG2	5:T:18:ARG:H	1.86	0.41
4:I:54:ILE:HG21	4:I:78:ALA:HB3	2.03	0.41
5:J:26:ARG:HD2	5:J:119:PHE:HD2	1.86	0.41
2:L:11:SER:HB2	2:L:21:ASN:ND2	2.36	0.41
5:E:37:LEU:HA	5:E:85:LEU:HD13	2.02	0.40
5:J:166:TYR:HB2	5:J:202:ARG:HG2	2.02	0.40
2:Q:12:ARG:HB3	2:Q:22:PHE:HB2	2.03	0.40
5:T:43:GLN:HB2	5:T:53:LEU:HD11	2.03	0.40
1:P:14:ARG:HB2	1:P:17:ARG:HB2	2.04	0.40
4:S:45:ASP:O	4:S:46:PRO:C	2.60	0.40
5:T:155:LYS:HE2	5:T:210:ARG:NH2	2.36	0.40
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.85	0.40
5:O:54:ILE:HD11	5:O:65:GLU:HG3	2.03	0.40
4:D:79:GLN:NE2	4:I:63:GLY:HA2	2.36	0.40
5:E:150:ILE:H	5:E:150:ILE:HG13	1.45	0.40
1:F:233:THR:HG23	1:F:243:LYS:HB2	2.04	0.40
4:N:40:LEU:HD23	4:N:52:LEU:HD13	2.04	0.40
5:O:81:PHE:HB3	5:O:83:PRO:HD2	2.02	0.40
4:S:15:GLU:HB3	4:S:16:GLY:H	1.62	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	268/278 (96%)	249 (93%)	17 (6%)	2 (1%)	22	55
1	F	269/278 (97%)	242 (90%)	26 (10%)	1 (0%)	34	66
1	K	268/278 (96%)	244 (91%)	24 (9%)	0	100	100
1	P	269/278 (97%)	246 (91%)	22 (8%)	1 (0%)	34	66
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	G	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	L	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	Q	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	D	199/207 (96%)	160 (80%)	35 (18%)	4 (2%)	7	33
4	I	200/207 (97%)	182 (91%)	17 (8%)	1 (0%)	29	61
4	N	200/207 (97%)	179 (90%)	18 (9%)	3 (2%)	10	38
4	S	199/207 (96%)	177 (89%)	16 (8%)	6 (3%)	4	25
5	E	241/246 (98%)	211 (88%)	27 (11%)	3 (1%)	13	43
5	J	241/246 (98%)	217 (90%)	21 (9%)	3 (1%)	13	43
5	O	241/246 (98%)	212 (88%)	25 (10%)	4 (2%)	9	36
5	T	241/246 (98%)	219 (91%)	19 (8%)	3 (1%)	13	43
All	All	3256/3360 (97%)	2930 (90%)	295 (9%)	31 (1%)	15	47

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ARG

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Mol	Chain	Res	Type
4	D	202	ALA
4	D	205	ASN
4	N	46	PRO
5	O	85	LEU
4	S	16	GLY
4	S	46	PRO
4	D	92	SER
4	D	186	ASP
5	E	123	GLY
5	O	86	HIS
4	S	63	GLY
4	S	74	GLY
5	T	196	PRO
4	S	48	GLU
5	T	115	ASN
1	P	53	GLU
5	E	169	HIS
4	I	136	ASP
5	J	108	ALA
5	O	46	LEU
4	S	184	SER
1	A	43	PRO
4	N	59	ALA
4	N	186	ASP
5	O	72	LEU
5	J	71	ILE
5	J	123	GLY
5	T	71	ILE
5	E	49	GLY
1	F	247	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	235/239 (98%)	228 (97%)	7 (3%)	41 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	235/239 (98%)	229 (97%)	6 (3%)	46 72
1	K	235/239 (98%)	225 (96%)	10 (4%)	29 61
1	P	236/239 (99%)	233 (99%)	3 (1%)	69 83
2	B	95/95 (100%)	92 (97%)	3 (3%)	39 68
2	G	95/95 (100%)	92 (97%)	3 (3%)	39 68
2	L	95/95 (100%)	95 (100%)	0	100 100
2	Q	95/95 (100%)	91 (96%)	4 (4%)	30 61
3	C	8/8 (100%)	8 (100%)	0	100 100
3	H	8/8 (100%)	8 (100%)	0	100 100
3	M	8/8 (100%)	6 (75%)	2 (25%)	0 2
3	R	8/8 (100%)	7 (88%)	1 (12%)	4 19
4	D	178/183 (97%)	174 (98%)	4 (2%)	52 76
4	I	179/183 (98%)	174 (97%)	5 (3%)	43 71
4	N	179/183 (98%)	174 (97%)	5 (3%)	43 71
4	S	178/183 (97%)	175 (98%)	3 (2%)	60 79
5	E	211/214 (99%)	200 (95%)	11 (5%)	23 55
5	J	211/214 (99%)	204 (97%)	7 (3%)	38 67
5	O	211/214 (99%)	202 (96%)	9 (4%)	29 61
5	T	211/214 (99%)	208 (99%)	3 (1%)	67 82
All	All	2911/2956 (98%)	2825 (97%)	86 (3%)	41 69

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	32	GLN
1	A	57	SER
1	A	86	ASN
1	A	87	GLN
1	A	196	ASP
1	A	203	CYS
2	B	48	LYS
2	B	70	PHE
2	B	80	CYS
4	D	65	LEU

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Mol	Chain	Res	Type
4	D	104	CYS
4	D	187	PHE
4	D	205	ASN
5	E	18	ARG
5	E	70	ASN
5	E	93	SER
5	E	114	SER
5	E	150	ILE
5	E	170	VAL
5	E	186	CYS
5	E	200	ASP
5	E	208	ARG
5	E	215	PHE
5	E	237	GLU
1	F	17	ARG
1	F	89	GLU
1	F	122	ASP
1	F	166	GLU
1	F	219	GLN
1	F	222	GLU
2	G	0	MET
2	G	9	VAL
2	G	45	ARG
4	I	65	LEU
4	I	147	SER
4	I	157	ASP
4	I	166	GLN
4	I	214	GLU
5	J	70	ASN
5	J	75	ARG
5	J	76	PHE
5	J	104	CYS
5	J	169	HIS
5	J	188	ASP
5	J	208	ARG
1	K	27	TYR
1	K	35	ARG
1	K	106	ASP
1	K	144	GLU
1	K	145	GLN
1	K	203	CYS
1	K	219	GLN

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Mol	Chain	Res	Type
1	K	229	GLU
1	K	235	PRO
1	K	273	ARG
3	M	5	ARG
3	M	9	LEU
4	N	3	GLN
4	N	4	LEU
4	N	116	LEU
4	N	178	CYS
4	N	208	ASN
5	O	37	LEU
5	O	70	ASN
5	O	75	ARG
5	O	85	LEU
5	O	202	ARG
5	O	228	GLN
5	O	236	ASP
5	O	242	ARG
5	O	251	SER
1	P	35	ARG
1	P	65	ARG
1	P	162	ASP
2	Q	12	ARG
2	Q	34	ASP
2	Q	42	ASN
2	Q	70	PHE
3	R	5	ARG
4	S	94	SER
4	S	143	ARG
4	S	180	LEU
5	T	169	HIS
5	T	186	CYS
5	T	228	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	145	GLN
2	B	83	ASN
5	E	79	GLN
5	E	177	ASN

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Mol	Chain	Res	Type
5	E	221	ASN
1	F	77	ASN
4	I	2	GLN
4	I	37	ASN
5	J	169	HIS
1	K	99	HIS
4	N	3	GLN
4	N	37	ASN
4	N	209	ASN
5	O	44	GLN
1	P	99	HIS
1	P	224	HIS
4	S	22	ASN
4	S	37	ASN
4	S	90	ASN
5	T	90	ASN
5	T	125	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	272/278 (97%)	0.18	6 (2%) 62 60	45, 73, 126, 144	0
1	F	272/278 (97%)	0.28	5 (1%) 68 67	59, 91, 120, 134	0
1	K	272/278 (97%)	0.91	50 (18%) 1 1	71, 106, 178, 201	0
1	P	272/278 (97%)	0.80	39 (14%) 2 2	61, 105, 171, 181	1 (0%)
2	B	100/100 (100%)	0.07	1 (1%) 82 83	59, 73, 94, 105	0
2	G	100/100 (100%)	0.18	1 (1%) 82 83	71, 92, 119, 130	0
2	L	100/100 (100%)	0.92	14 (14%) 2 2	98, 133, 158, 164	0
2	Q	100/100 (100%)	0.91	10 (10%) 7 7	92, 129, 155, 162	0
3	C	9/9 (100%)	0.09	0 100 100	43, 47, 52, 60	0
3	H	9/9 (100%)	0.11	0 100 100	60, 60, 65, 71	0
3	M	9/9 (100%)	0.28	0 100 100	71, 72, 75, 88	0
3	R	9/9 (100%)	0.35	0 100 100	65, 67, 70, 80	0
4	D	201/207 (97%)	0.60	19 (9%) 8 9	46, 81, 168, 175	0
4	I	202/207 (97%)	0.10	2 (0%) 82 83	39, 64, 102, 115	0
4	N	202/207 (97%)	0.18	1 (0%) 91 91	50, 78, 117, 132	0
4	S	201/207 (97%)	0.65	19 (9%) 8 9	52, 88, 166, 186	0
5	E	243/246 (98%)	0.50	18 (7%) 14 15	55, 111, 143, 153	0
5	J	243/246 (98%)	0.07	0 100 100	38, 60, 91, 109	0
5	O	243/246 (98%)	0.15	0 100 100	37, 76, 109, 126	0
5	T	243/246 (98%)	0.56	14 (5%) 23 24	50, 103, 140, 152	0
All	All	3302/3360 (98%)	0.43	199 (6%) 21 22	37, 89, 160, 201	1 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S	147	SER	9.4
4	S	185	MET	8.2
1	P	199	ALA	6.2
1	K	195	SER	6.0
1	K	194	ILE	6.0
1	K	191	HIS	6.0
1	K	190	THR	5.5
1	K	205	ALA	5.4
1	K	216	THR	5.3
4	S	182	MET	5.2
2	L	0	MET	5.1
1	P	201	LEU	5.1
1	K	230	LEU	5.0
4	S	184	SER	5.0
4	S	183	ARG	5.0
4	D	195	TRP	4.8
1	K	188	HIS	4.7
1	P	276	PRO	4.7
1	K	248	VAL	4.6
2	L	1	ILE	4.5
4	D	154	LEU	4.5
1	P	225	THR	4.5
1	K	274	TRP	4.4
5	E	158	LEU	4.4
1	K	189	VAL	4.4
1	K	218	GLN	4.4
1	P	250	PRO	4.4
4	D	147	SER	4.3
1	P	249	VAL	4.3
5	E	143	PHE	4.2
1	K	271	THR	4.2
2	Q	40	LEU	4.2
1	K	262	GLN	4.1
4	S	154	LEU	4.1
4	D	149	ASP	4.1
4	S	195	TRP	4.1
1	P	205	ALA	4.0
2	Q	48	LYS	4.0
1	K	192	HIS	4.0
1	K	225	THR	4.0
2	Q	79	ALA	4.0
4	D	215	ASP	4.0
1	P	260	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	15	ALA	3.8
4	D	174	ILE	3.8
1	P	254	GLU	3.7
1	P	224	HIS	3.7
5	E	178	GLY	3.7
1	K	187	THR	3.7
1	P	187	THR	3.7
2	Q	92	ILE	3.6
4	D	193	VAL	3.6
1	P	272	LEU	3.6
1	K	201	LEU	3.5
1	K	258	THR	3.5
4	D	145	SER	3.5
5	E	138	PRO	3.5
5	E	258	ALA	3.5
1	K	264	GLU	3.5
1	P	189	VAL	3.4
4	D	148	SER	3.3
4	D	157	ASP	3.3
1	K	245	ALA	3.3
1	K	270	VAL	3.3
1	K	261	VAL	3.3
1	P	251	SER	3.3
1	P	259	CYS	3.2
5	T	197	ALA	3.2
1	P	186	LYS	3.2
1	K	260	HIS	3.2
1	K	223	GLY	3.2
1	P	194	ILE	3.2
1	K	217	TRP	3.2
5	T	224	ARG	3.1
1	K	203	CYS	3.1
2	L	99	MET	3.1
1	P	218	GLN	3.1
1	K	226	GLN	3.1
4	D	210	SER	3.1
1	F	273	ARG	3.1
5	E	177	ASN	3.0
5	E	162	ALA	3.0
1	P	248	VAL	3.0
5	T	245	PRO	3.0
1	K	244	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	205	ASN	2.9
1	K	193	PRO	2.9
1	K	219	GLN	2.9
5	T	138	PRO	2.9
1	F	201	LEU	2.9
5	T	204	ALA	2.8
1	P	270	VAL	2.8
5	T	142	VAL	2.8
4	D	219	PRO	2.8
5	T	113	SER	2.8
1	K	247	VAL	2.8
1	K	224	HIS	2.8
1	A	253	GLU	2.8
1	P	275	LYS	2.8
1	K	228	THR	2.7
1	P	203	CYS	2.7
5	E	141	ALA	2.7
1	K	204	TRP	2.6
4	S	151	SER	2.6
2	L	42	ASN	2.6
2	Q	80	CYS	2.6
1	K	275	LYS	2.6
1	A	197	HIS	2.6
1	P	179	LEU	2.6
5	E	198	LEU	2.6
2	L	27	VAL	2.6
1	P	215	LEU	2.5
4	S	205	ASN	2.5
1	K	215	LEU	2.5
1	A	273	ARG	2.5
5	T	114	SER	2.5
4	S	207	PHE	2.5
1	K	196	ASP	2.5
1	K	85	TYR	2.5
5	E	142	VAL	2.5
1	K	227	ASP	2.5
4	S	193	VAL	2.4
1	K	255	GLN	2.4
4	S	174	ILE	2.4
1	K	276	PRO	2.4
1	P	243	LYS	2.4
5	T	116	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	Q	44	GLU	2.4
1	P	230	LEU	2.4
1	K	259	CYS	2.4
4	I	147	SER	2.4
2	L	18	GLY	2.4
4	S	149	ASP	2.4
1	P	256	ARG	2.3
5	E	197	ALA	2.3
1	K	243	LYS	2.3
1	K	256	ARG	2.3
1	P	185	PRO	2.3
5	T	200	ASP	2.3
2	Q	23	LEU	2.3
4	S	148	SER	2.3
2	L	97	ARG	2.3
2	Q	24	ASN	2.3
5	E	94	LEU	2.3
1	A	226	GLN	2.3
5	T	178	GLY	2.3
5	E	253	GLU	2.3
1	P	190	THR	2.3
2	L	82	VAL	2.3
2	Q	42	ASN	2.3
1	P	198	GLU	2.3
2	Q	68	THR	2.3
4	D	214	GLU	2.3
1	K	202	ARG	2.3
5	T	115	ASN	2.3
5	E	46	LEU	2.3
5	T	158	LEU	2.3
1	P	204	TRP	2.2
1	P	197	HIS	2.2
4	D	165	SER	2.2
1	K	257	TYR	2.2
1	P	191	HIS	2.2
2	L	98	ASP	2.2
1	K	249	VAL	2.2
1	F	104	GLY	2.2
1	K	269	PRO	2.2
1	P	94	THR	2.2
1	F	217	TRP	2.2
4	D	161	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
4	S	145	SER	2.2
5	E	223	PHE	2.1
1	P	227	ASP	2.1
5	E	193	LYS	2.1
1	P	138	THR	2.1
1	P	273	ARG	2.1
4	N	139	VAL	2.1
1	P	212	GLU	2.1
2	L	39	LEU	2.1
5	T	85	LEU	2.1
5	E	137	PRO	2.1
5	E	192	LEU	2.1
4	D	203	CYS	2.1
4	D	164	VAL	2.1
2	L	14	PRO	2.1
4	S	165	SER	2.1
1	A	196	ASP	2.1
4	I	149	ASP	2.1
1	P	228	THR	2.1
4	S	180	LEU	2.0
4	D	184	SER	2.0
2	L	83	ASN	2.0
1	F	274	TRP	2.0
1	A	257	TYR	2.0
4	S	173	TYR	2.0
2	G	88	SER	2.0
4	S	167	SER	2.0
1	K	41	ALA	2.0
2	B	1	ILE	2.0
2	L	81	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.