Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:45 AM GMT

PDB ID	:	2ICW
Title	:	Crystal structure of a complete ternary complex between TCR, superantigen, and peptide-MHC class II molecule
Authors	:	Wang, L.; Zhao, Y.; Li, H.
Deposited on	:	2006-09-13
Resolution	:	2.41 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

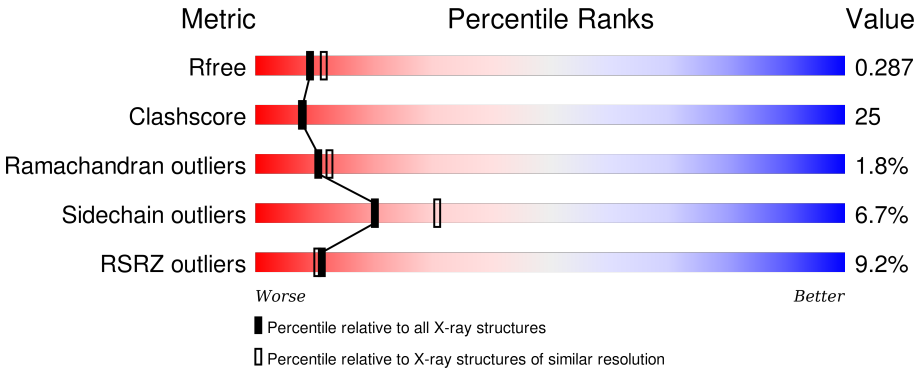
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	179	62% 34%
1	D	179	2% 65% 31%
2	B	190	14% 54% 38% 5%
2	E	190	9% 54% 38% 5%
3	C	13	54% 38% 8%

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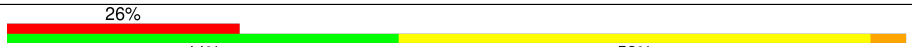
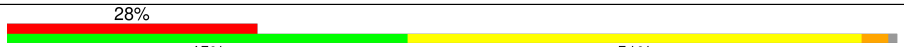
Mol	Chain	Length	Quality of chain
3	F	13	
4	G	213	
4	H	213	
5	I	110	
5	K	110	
6	J	113	
6	L	113	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13464 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	Se	0	0	0
			1474	954	239	276	2	3			
1	D	179	Total	C	N	O	S	Se	0	0	0
			1474	954	239	276	2	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MSE	MET	MODIFIED RESIDUE	UNP P01903
A	36	MSE	MET	MODIFIED RESIDUE	UNP P01903
A	73	MSE	MET	MODIFIED RESIDUE	UNP P01903
D	23	MSE	MET	MODIFIED RESIDUE	UNP P01903
D	36	MSE	MET	MODIFIED RESIDUE	UNP P01903
D	73	MSE	MET	MODIFIED RESIDUE	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1504	946	267	285	6			
2	E	185	Total	C	N	O	S	0	0	0
			1513	951	269	287	6			

- Molecule 3 is a protein called haemagglutinin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			
3	F	13	Total	C	N	O	0	0	0
			106	69	18	19			

- Molecule 4 is a protein called Mycoplasma arthritidis mitogen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	213	Total	C	N	O	S	0	0	0
			1786	1154	301	326	5			
4	H	213	Total	C	N	O	S	0	0	0
			1786	1154	301	326	5			

- Molecule 5 is a protein called T-cell receptor alpha chain V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	110	Total	C	N	O	S	0	1	0
			863	557	144	160	2			
5	K	109	Total	C	N	O	S	0	0	0
			847	545	142	158	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	43	PRO	LEU	ENGINEERED	UNP P01738
I	82	ARG	TRP	ENGINEERED	UNP P01738
K	43	PRO	LEU	ENGINEERED	UNP P01738
K	82	ARG	TRP	ENGINEERED	UNP P01738

- Molecule 6 is a protein called T-cell receptor beta chain V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	113	Total	C	N	O	S	0	0	0
			857	528	151	175	3			
6	L	111	Total	C	N	O	S	0	0	0
			843	520	149	171	3			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	10	ASN	SER	SEE REMARK 999	UNP P04213
J	17	GLU	GLY	ENGINEERED	UNP P04213
J	24	ASN	HIS	SEE REMARK 999	UNP P04213
J	30	ASN	ASP	SEE REMARK 999	UNP P04213
J	31	ASN	TYR	SEE REMARK 999	UNP P04213
J	42	GLU	GLY	ENGINEERED	UNP P04213
J	51	GLY	VAL	SEE REMARK 999	UNP P04213
J	53	GLY	ASP	SEE REMARK 999	UNP P04213
J	80	SER	LEU	ENGINEERED	UNP P04213
J	81	ALA	-	SEE REMARK 999	UNP P04213
J	82	THR	-	SEE REMARK 999	UNP P04213

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Chain	Residue	Modelled	Actual	Comment	Reference
J	83	PRO	-	SEE REMARK 999	UNP P04213
J	84	SER	-	SEE REMARK 999	UNP P04213
J	85	GLN	-	SEE REMARK 999	UNP P04213
J	86	THR	-	SEE REMARK 999	UNP P04213
J	87	SER	-	SEE REMARK 999	UNP P04213
J	88	VAL	-	SEE REMARK 999	UNP P04213
J	89	TYR	-	SEE REMARK 999	UNP P04213
J	90	PHE	-	SEE REMARK 999	UNP P04213
J	91	CYS	-	SEE REMARK 999	UNP P04213
J	92	ALA	-	SEE REMARK 999	UNP P04213
J	93	SER	-	SEE REMARK 999	UNP P04213
J	94	GLY	-	SEE REMARK 999	UNP P04213
J	95	GLY	-	SEE REMARK 999	UNP P04213
J	96	GLY	-	SEE REMARK 999	UNP P04213
J	97	GLY	-	SEE REMARK 999	UNP P04213
J	98	THR	-	SEE REMARK 999	UNP P04213
J	100	TYR	-	SEE REMARK 999	UNP P04213
J	101	PHE	-	SEE REMARK 999	UNP P04213
J	102	GLY	-	SEE REMARK 999	UNP P04213
J	103	ALA	-	SEE REMARK 999	UNP P04213
J	104	GLY	-	SEE REMARK 999	UNP P04213
J	105	THR	-	SEE REMARK 999	UNP P04213
J	106	ARG	-	SEE REMARK 999	UNP P04213
J	107	LEU	-	SEE REMARK 999	UNP P04213
J	108	SER	-	SEE REMARK 999	UNP P04213
J	109	VAL	-	SEE REMARK 999	UNP P04213
J	110	LEU	-	SEE REMARK 999	UNP P04213
J	111	SER	-	CLONING ARTIFACT	UNP P04213
J	112	SER	-	CLONING ARTIFACT	UNP P04213
J	113	ALA	-	CLONING ARTIFACT	UNP P04213
L	10	ASN	SER	SEE REMARK 999	UNP P04213
L	17	GLU	GLY	ENGINEERED	UNP P04213
L	24	ASN	HIS	SEE REMARK 999	UNP P04213
L	30	ASN	ASP	SEE REMARK 999	UNP P04213
L	31	ASN	TYR	SEE REMARK 999	UNP P04213
L	42	GLU	GLY	ENGINEERED	UNP P04213
L	51	GLY	VAL	SEE REMARK 999	UNP P04213
L	53	GLY	ASP	SEE REMARK 999	UNP P04213
L	80	SER	LEU	ENGINEERED	UNP P04213
L	81	ALA	-	SEE REMARK 999	UNP P04213
L	82	THR	-	SEE REMARK 999	UNP P04213
L	83	PRO	-	SEE REMARK 999	UNP P04213

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Chain	Residue	Modelled	Actual	Comment	Reference
L	84	SER	-	SEE REMARK 999	UNP P04213
L	85	GLN	-	SEE REMARK 999	UNP P04213
L	86	THR	-	SEE REMARK 999	UNP P04213
L	87	SER	-	SEE REMARK 999	UNP P04213
L	88	VAL	-	SEE REMARK 999	UNP P04213
L	89	TYR	-	SEE REMARK 999	UNP P04213
L	90	PHE	-	SEE REMARK 999	UNP P04213
L	91	CYS	-	SEE REMARK 999	UNP P04213
L	92	ALA	-	SEE REMARK 999	UNP P04213
L	93	SER	-	SEE REMARK 999	UNP P04213
L	94	GLY	-	SEE REMARK 999	UNP P04213
L	95	GLY	-	SEE REMARK 999	UNP P04213
L	96	GLY	-	SEE REMARK 999	UNP P04213
L	97	GLY	-	SEE REMARK 999	UNP P04213
L	98	THR	-	SEE REMARK 999	UNP P04213
L	100	TYR	-	SEE REMARK 999	UNP P04213
L	101	PHE	-	SEE REMARK 999	UNP P04213
L	102	GLY	-	SEE REMARK 999	UNP P04213
L	103	ALA	-	SEE REMARK 999	UNP P04213
L	104	GLY	-	SEE REMARK 999	UNP P04213
L	105	THR	-	SEE REMARK 999	UNP P04213
L	106	ARG	-	SEE REMARK 999	UNP P04213
L	107	LEU	-	SEE REMARK 999	UNP P04213
L	108	SER	-	SEE REMARK 999	UNP P04213
L	109	VAL	-	SEE REMARK 999	UNP P04213
L	110	LEU	-	SEE REMARK 999	UNP P04213
L	111	SER	-	CLONING ARTIFACT	UNP P04213
L	112	SER	-	CLONING ARTIFACT	UNP P04213
L	113	ALA	-	CLONING ARTIFACT	UNP P04213

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	59	Total O 59 59	0	0
7	B	38	Total O 38 38	0	0
7	C	8	Total O 8 8	0	0
7	D	67	Total O 67 67	0	0
7	E	34	Total O 34 34	0	0

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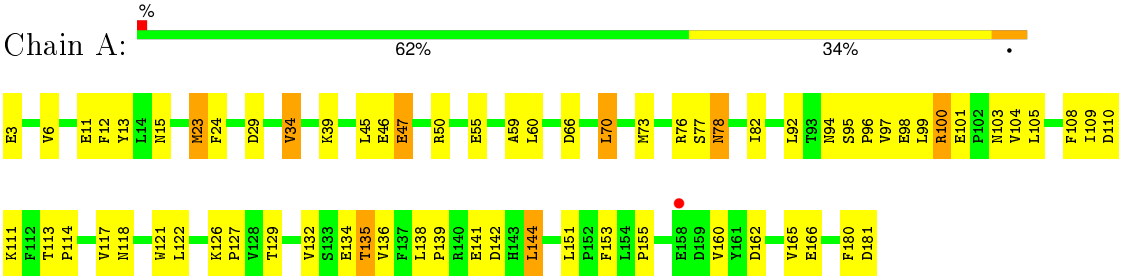
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	8	Total O 8 8	0	0
7	G	32	Total O 32 32	0	0
7	H	38	Total O 38 38	0	0
7	I	1	Total O 1 1	0	0
7	J	8	Total O 8 8	0	0
7	K	4	Total O 4 4	0	0
7	L	8	Total O 8 8	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

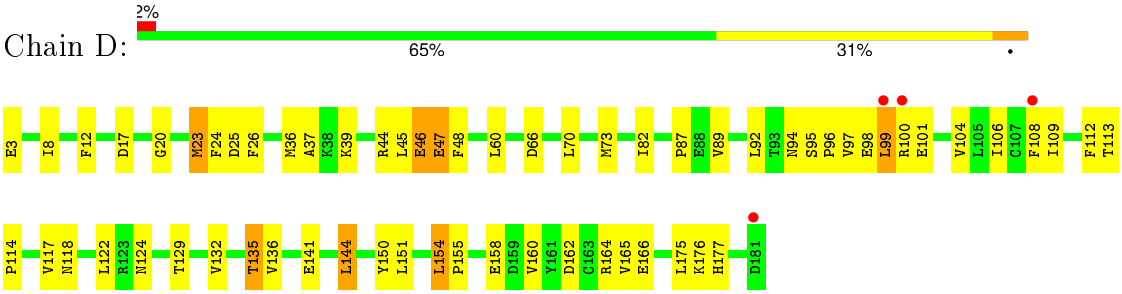
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



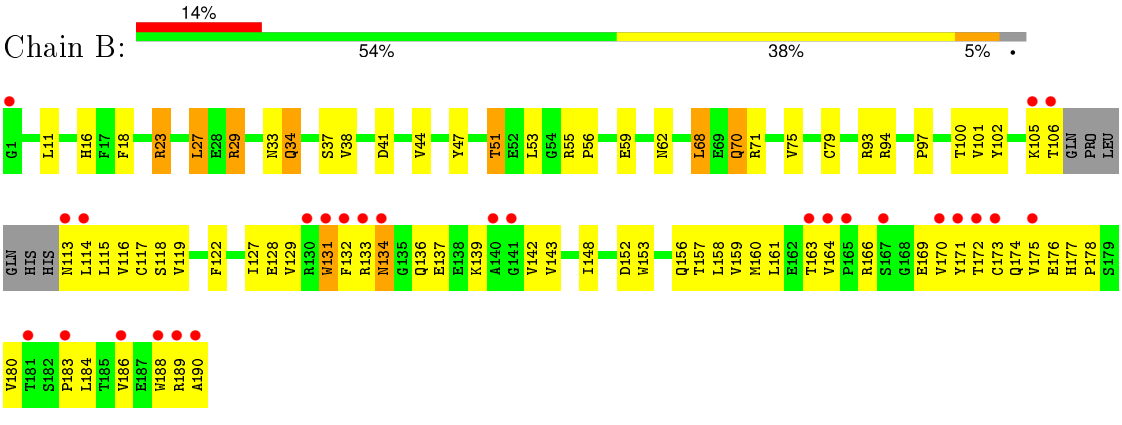
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain D:



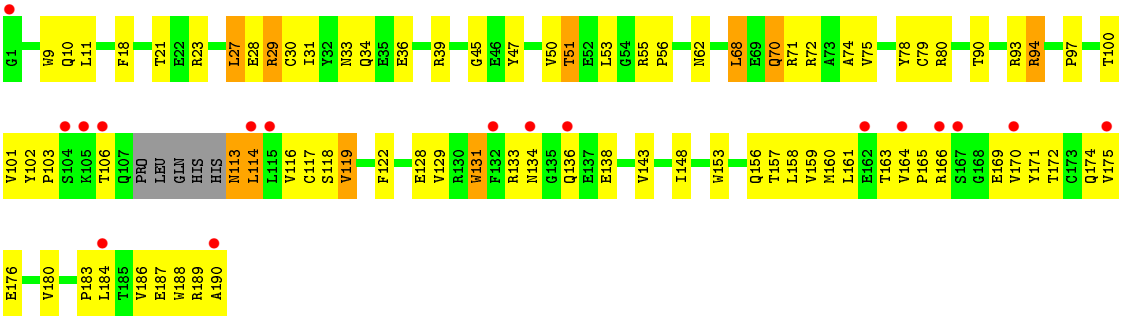
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain B:



- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain E:



- Molecule 3: haemagglutinin peptide

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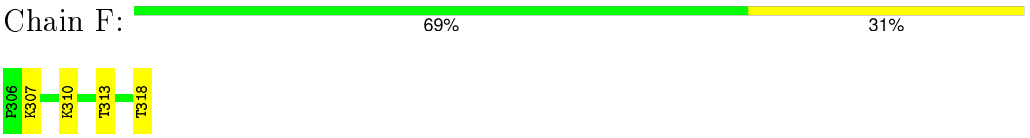
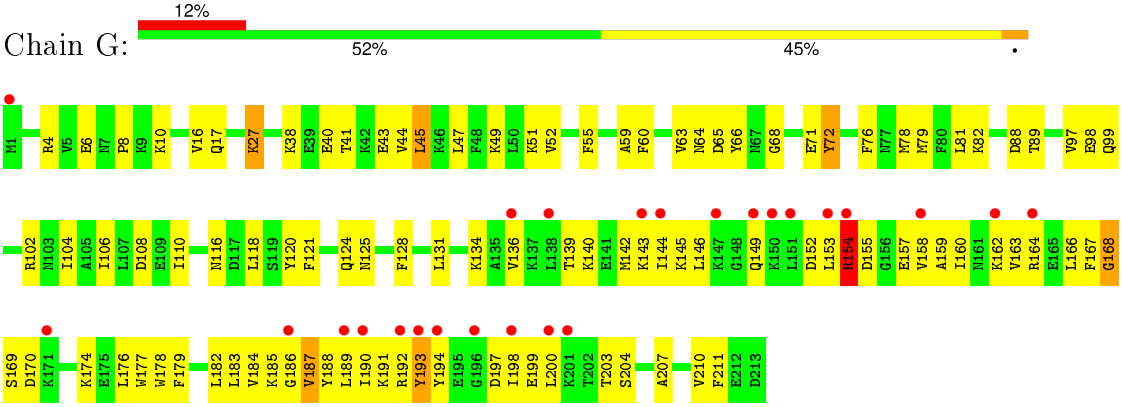
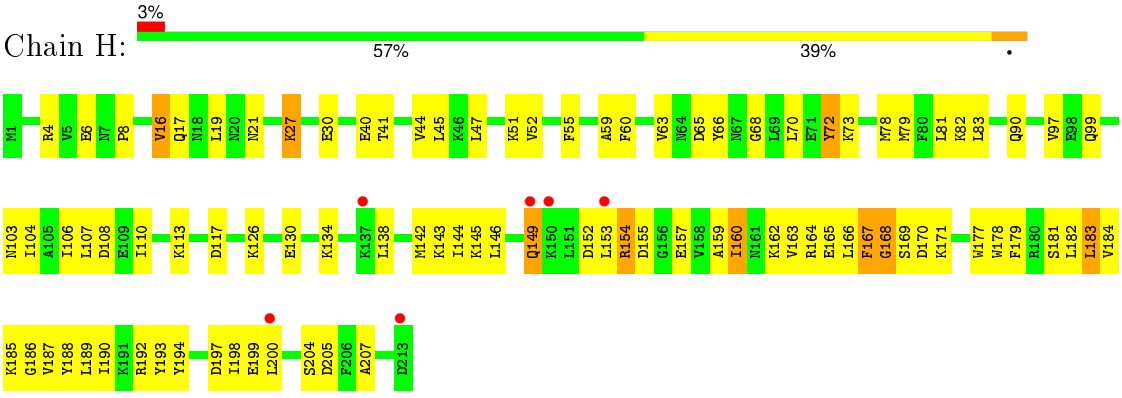


- Molecule 4: Mycoplasma arthritidis mitogen

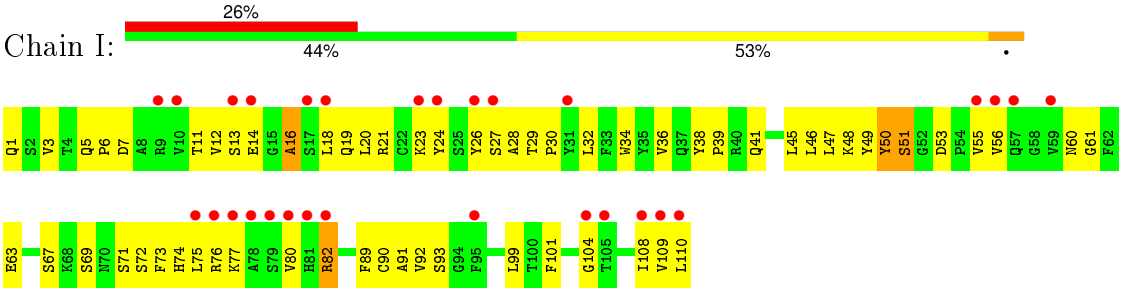


- Molecule 4: Mycoplasma arthritidis mitogen



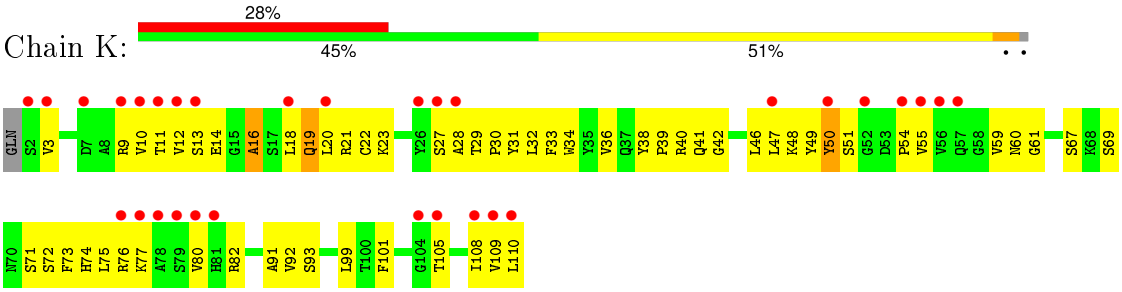
• Molecule 5: T-cell receptor alpha chain V

Chain I:



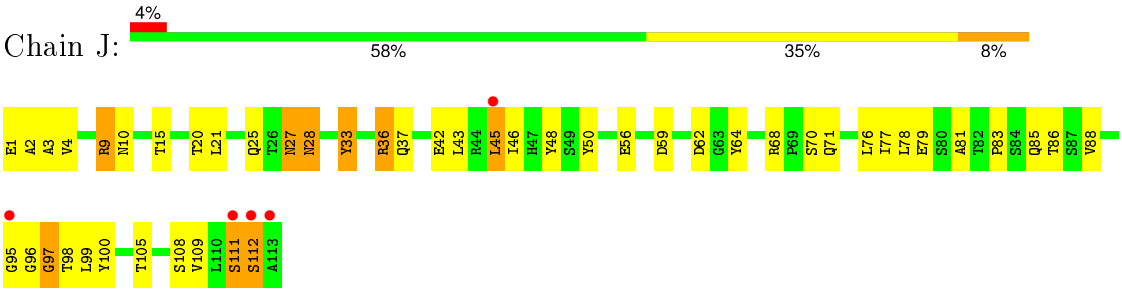
• Molecule 5: T-cell receptor alpha chain V

Chain K:



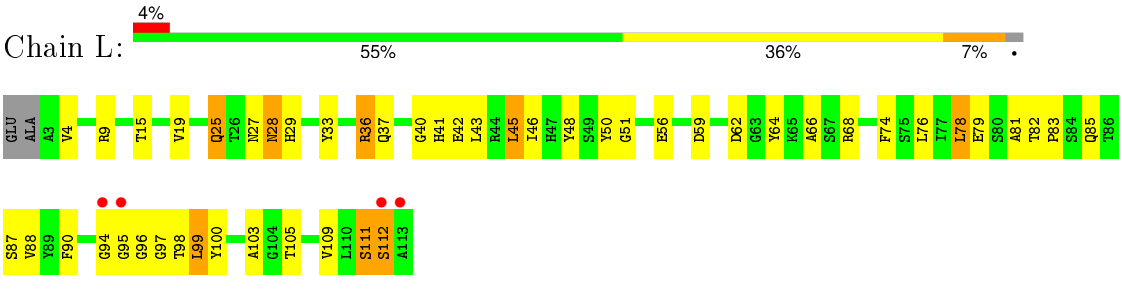
• Molecule 6: T-cell receptor beta chain V

Chain J:



• Molecule 6: T-cell receptor beta chain V

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.52Å 86.82Å 116.98Å 110.27° 92.32° 107.87°	Depositor
Resolution (Å)	47.79 – 2.41 47.79 – 2.41	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.79-2.41) 83.5 (47.79-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.42Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.288 0.241 , 0.287	Depositor DCC
R_{free} test set	3944 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 78299 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13464	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/1516	0.68	0/2061
1	D	0.43	0/1516	0.69	0/2061
2	B	0.41	0/1540	0.65	0/2088
2	E	0.41	0/1549	0.65	0/2100
3	C	0.43	0/107	0.71	0/141
3	F	0.52	0/107	0.73	0/141
4	G	0.40	0/1816	0.56	0/2431
4	H	0.41	0/1816	0.56	0/2431
5	I	0.35	0/891	0.56	0/1209
5	K	0.33	0/870	0.57	0/1181
6	J	0.36	0/875	0.63	0/1185
6	L	0.37	0/861	0.66	0/1166
All	All	0.40	0/13464	0.62	0/18195

There are no bond length outliers.

There are no bond angle outliers.

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	1474	0	1407	55	0
1	D	1474	0	1407	56	0
2	B	1504	0	1439	85	0
2	E	1513	0	1447	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	106	0	119	6	0
3	F	106	0	119	2	0
4	G	1786	0	1831	102	0
4	H	1786	0	1831	103	0
5	I	863	0	839	63	0
5	K	847	0	823	56	0
6	J	857	0	811	56	0
6	L	843	0	797	43	0
7	A	59	0	0	2	0
7	B	38	0	0	0	0
7	C	8	0	0	0	0
7	D	67	0	0	1	0
7	E	34	0	0	1	0
7	F	8	0	0	0	0
7	G	32	0	0	3	0
7	H	38	0	0	1	0
7	I	1	0	0	0	0
7	J	8	0	0	0	0
7	K	4	0	0	0	0
7	L	8	0	0	0	0
All	All	13464	0	12870	644	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 25.

All (644) 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:H:160:ILE:HD13	4:H:160:ILE:H	1.15	1.09
4:G:154:ARG:HD3	4:G:154:ARG:H	1.21	1.00
2:B:116:VAL:HG12	2:B:160:MET:HG2	1.40	0.99
5:K:99:LEU:HG	6:L:99:LEU:HD23	1.47	0.96
4:H:51:LYS:HG3	4:H:104:ILE:HG23	1.47	0.96
1:A:99:LEU:H	1:A:99:LEU:HD12	1.31	0.94
6:J:64:TYR:CD1	6:J:78:LEU:HD21	2.02	0.94
4:H:44:VAL:HA	4:H:47:LEU:HD23	1.49	0.93
5:K:11:THR:HG22	5:K:108:ILE:HB	1.50	0.92
2:B:71:ARG:HH11	3:C:314:LEU:HD11	1.35	0.92
4:H:60:PHE:HA	4:H:63:VAL:HG12	1.51	0.91
1:D:73:MSE:HE1	2:E:53:LEU:HB3	1.52	0.90
1:D:99:LEU:H	1:D:99:LEU:HD12	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:51:LYS:HG3	4:G:104:ILE:HG23	1.53	0.88
2:E:47:TYR:H	2:E:62:ASN:HD21	1.22	0.87
3:C:307:LYS:HD3	3:C:307:LYS:H	1.38	0.87
2:B:47:TYR:H	2:B:62:ASN:HD21	1.20	0.86
6:J:37:GLN:HB2	6:J:43:LEU:HD13	1.60	0.84
6:L:37:GLN:HB2	6:L:43:LEU:HD13	1.60	0.83
1:A:23:MSE:HE1	1:A:138:LEU:HA	1.61	0.83
2:E:68:LEU:O	2:E:72:ARG:HG3	1.78	0.82
4:G:44:VAL:HA	4:G:47:LEU:HD23	1.60	0.82
2:E:116:VAL:HG12	2:E:160:MET:HG2	1.62	0.81
4:H:157:GLU:HA	4:H:160:ILE:HD11	1.62	0.80
4:G:63:VAL:HG23	4:G:72:TYR:HE1	1.46	0.80
2:B:131:TRP:NE1	2:B:161:LEU:HB2	1.97	0.80
1:D:92:LEU:HG	1:D:108:PHE:HE2	1.45	0.79
4:G:63:VAL:HG23	4:G:72:TYR:CE1	2.16	0.79
4:H:192:ARG:HB3	4:H:192:ARG:NH1	1.98	0.78
1:D:23:MSE:HG2	1:D:24:PHE:N	1.98	0.78
1:D:39:LYS:HG3	4:H:106:ILE:HD13	1.65	0.78
4:H:160:ILE:CD1	4:H:160:ILE:H	1.95	0.78
4:H:179:PHE:O	4:H:183:LEU:HD22	1.82	0.78
4:G:157:GLU:HB2	4:G:160:ILE:HG22	1.66	0.78
2:E:113:ASN:HB3	2:E:163:THR:HG23	1.64	0.77
2:E:170:VAL:HG22	2:E:189:ARG:HE	1.50	0.77
4:G:152:ASP:O	4:G:158:VAL:HG21	1.83	0.77
4:H:192:ARG:HB3	4:H:192:ARG:HH11	1.50	0.77
5:I:99:LEU:HG	6:J:99:LEU:HD23	1.67	0.76
4:G:154:ARG:CD	4:G:154:ARG:H	1.97	0.76
2:E:172:THR:HG22	2:E:187:GLU:HG2	1.67	0.76
4:H:160:ILE:HG21	6:L:28:ASN:HB2	1.67	0.76
4:H:160:ILE:N	4:H:160:ILE:HD13	1.99	0.75
2:E:166:ARG:HG2	2:E:169:GLU:HG3	1.69	0.75
4:G:16:VAL:HG21	4:G:81:LEU:HD11	1.69	0.75
5:I:45:LEU:HD22	6:J:98:THR:HG21	1.68	0.74
1:A:98:GLU:O	1:A:101:GLU:HB2	1.86	0.74
6:J:3:ALA:HB1	6:J:27:ASN:HD21	1.51	0.74
1:A:39:LYS:HG3	4:G:106:ILE:HD13	1.70	0.74
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.68	0.73
5:K:48:LYS:HE3	5:K:50:TYR:HE1	1.53	0.73
4:H:70:LEU:H	4:H:70:LEU:HD12	1.52	0.73
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.68	0.73
4:H:184:VAL:O	4:H:187:VAL:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:154:ARG:HH21	5:K:59:VAL:HG21	1.53	0.72
4:H:192:ARG:NH1	4:H:200:LEU:HD21	2.04	0.72
5:I:82:ARG:HB3	5:I:82:ARG:HH21	1.53	0.72
1:D:95:SER:HB2	1:D:96:PRO:HD2	1.71	0.71
4:G:192:ARG:HH22	6:J:97:GLY:N	1.87	0.71
4:H:192:ARG:HH22	5:K:50:TYR:HB3	1.55	0.71
1:A:23:MSE:HE1	1:A:139:PRO:HD3	1.72	0.70
5:I:82:ARG:CB	5:I:82:ARG:HH21	2.04	0.70
1:D:39:LYS:HG3	4:H:106:ILE:CD1	2.20	0.70
2:B:127:ILE:HG13	2:B:177:HIS:HB2	1.73	0.70
4:G:162:LYS:O	4:G:166:LEU:HD13	1.92	0.70
6:J:27:ASN:N	6:J:27:ASN:HD22	1.86	0.70
1:A:144:LEU:HD13	2:B:34:GLN:NE2	2.07	0.69
5:I:32:LEU:HD13	5:I:73:PHE:HB2	1.73	0.69
6:L:36:ARG:NH2	6:L:85:GLN:HA	2.07	0.69
4:H:193:TYR:HB2	4:H:200:LEU:HD12	1.74	0.69
2:B:180:VAL:HG21	2:B:184:LEU:HD13	1.75	0.69
4:H:186:GLY:O	4:H:190:ILE:HD13	1.93	0.68
6:L:36:ARG:HB3	6:L:46:ILE:HD11	1.74	0.68
5:K:21:ARG:HA	5:K:74:HIS:ND1	2.07	0.68
1:D:39:LYS:HE3	1:D:60:LEU:HD13	1.75	0.68
4:G:157:GLU:HB2	4:G:160:ILE:CG2	2.23	0.68
4:H:162:LYS:O	4:H:166:LEU:HD13	1.94	0.68
4:G:60:PHE:HA	4:G:63:VAL:HG12	1.76	0.68
4:H:160:ILE:HG21	6:L:28:ASN:CB	2.23	0.67
4:H:51:LYS:CG	4:H:104:ILE:HG23	2.23	0.67
5:K:32:LEU:HD13	5:K:73:PHE:HB2	1.75	0.67
6:J:64:TYR:CE1	6:J:78:LEU:HD21	2.29	0.67
4:G:153:LEU:HG	4:G:191:LYS:HZ2	1.58	0.67
6:J:9:ARG:HD2	6:J:9:ARG:H	1.60	0.66
4:H:51:LYS:HE3	4:H:108:ASP:OD1	1.95	0.66
4:H:60:PHE:HA	4:H:63:VAL:CG1	2.22	0.66
5:K:49:TYR:HE2	5:K:54:PRO:HA	1.61	0.66
4:G:177:TRP:CH2	6:J:28:ASN:HA	2.30	0.66
1:D:97:VAL:O	1:D:98:GLU:HG3	1.95	0.66
6:J:36:ARG:NH2	6:J:85:GLN:HA	2.11	0.66
6:J:45:LEU:HD11	6:J:59:ASP:OD2	1.95	0.66
4:H:16:VAL:HG21	4:H:81:LEU:HD11	1.77	0.66
4:H:199:GLU:HG3	5:K:51:SER:HB3	1.78	0.65
1:D:99:LEU:N	1:D:99:LEU:HD12	2.11	0.65
4:H:154:ARG:HH21	5:K:59:VAL:CG2	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:VAL:HG21	2:B:184:LEU:CD1	2.26	0.65
2:B:176:GLU:HG3	2:B:183:PRO:HB3	1.79	0.65
6:J:96:GLY:O	6:J:98:THR:N	2.29	0.65
2:B:71:ARG:HH11	3:C:314:LEU:CD1	2.10	0.65
1:A:3:GLU:HA	2:B:18:PHE:CD2	2.32	0.64
5:I:101:PHE:CD2	6:J:43:LEU:HB2	2.32	0.64
4:H:142:MET:SD	4:H:187:VAL:HG12	2.37	0.64
5:I:61:GLY:O	5:I:77:LYS:HG3	1.97	0.64
4:H:192:ARG:NH2	5:K:50:TYR:HB3	2.12	0.64
5:K:61:GLY:O	5:K:77:LYS:HG3	1.97	0.64
2:E:27:LEU:HD13	2:E:29:ARG:HD3	1.80	0.64
6:J:45:LEU:HD12	6:J:45:LEU:H	1.62	0.64
1:A:23:MSE:HG2	1:A:24:PHE:N	2.13	0.63
4:G:192:ARG:HH22	6:J:96:GLY:C	2.02	0.63
2:B:134:ASN:HB3	2:B:170:VAL:HB	1.79	0.63
4:G:153:LEU:O	4:G:155:ASP:N	2.31	0.63
2:B:131:TRP:CD1	2:B:161:LEU:HB2	2.32	0.63
6:L:96:GLY:O	6:L:98:THR:N	2.32	0.63
6:J:36:ARG:HB3	6:J:46:ILE:HD11	1.81	0.63
1:D:99:LEU:HA	1:D:155:PRO:HB2	1.81	0.62
3:C:307:LYS:HD3	3:C:307:LYS:N	2.11	0.62
6:L:64:TYR:HD1	6:L:78:LEU:HD22	1.64	0.62
2:E:97:PRO:HB2	2:E:119:VAL:HG23	1.81	0.62
1:A:99:LEU:H	1:A:99:LEU:CD1	2.10	0.62
4:G:45:LEU:HD22	4:G:49:LYS:HE3	1.80	0.62
5:I:11:THR:HG22	5:I:108:ILE:HB	1.82	0.62
1:A:132:VAL:HG12	1:A:151:LEU:HD23	1.81	0.62
2:E:143:VAL:HG13	2:E:160:MET:HB2	1.81	0.62
6:J:45:LEU:N	6:J:45:LEU:HD12	2.13	0.62
4:H:134:LYS:HE2	4:H:138:LEU:HD11	1.82	0.62
5:I:46:LEU:HD12	5:I:47:LEU:HG	1.82	0.62
2:B:131:TRP:CZ3	2:B:173:CYS:HB2	2.35	0.62
4:G:4:ARG:HD3	4:G:118:LEU:HD23	1.81	0.62
4:H:106:ILE:O	4:H:110:ILE:HG13	2.00	0.62
1:D:23:MSE:O	1:D:23:MSE:HE2	2.00	0.61
2:E:180:VAL:HG21	2:E:184:LEU:CD1	2.30	0.61
4:H:192:ARG:HH11	4:H:192:ARG:CB	2.11	0.61
2:B:105:LYS:O	2:B:106:THR:HG23	1.99	0.61
1:D:66:ASP:OD2	3:F:313:THR:HG21	2.01	0.61
4:H:177:TRP:CH2	6:L:28:ASN:HA	2.34	0.61
1:D:117:VAL:HG23	1:D:166:GLU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:4:VAL:HG21	6:L:100:TYR:O	2.01	0.61
4:G:59:ALA:HA	4:G:79:MET:HE1	1.81	0.61
6:L:111:SER:O	6:L:112:SER:HB3	2.00	0.61
6:J:4:VAL:HG21	6:J:100:TYR:O	2.00	0.61
5:I:45:LEU:CD2	6:J:98:THR:HG21	2.30	0.61
4:G:155:ASP:O	4:G:158:VAL:HG23	2.01	0.60
5:K:32:LEU:HD23	5:K:92:VAL:HG12	1.84	0.60
2:B:55:ARG:O	2:B:59:GLU:HG3	2.01	0.60
5:I:91:ALA:HB2	5:I:101:PHE:HA	1.84	0.59
2:B:97:PRO:HB2	2:B:119:VAL:CG2	2.32	0.59
4:G:153:LEU:HD13	5:I:48:LYS:NZ	2.17	0.59
2:E:97:PRO:HB3	2:E:122:PHE:HB3	1.84	0.59
4:G:40:GLU:CD	4:G:40:GLU:H	2.04	0.59
2:E:29:ARG:HD2	2:E:36:GLU:OE2	2.02	0.59
4:H:134:LYS:O	4:H:138:LEU:HG	2.02	0.59
4:H:60:PHE:CA	4:H:63:VAL:HG12	2.28	0.59
4:H:16:VAL:HG21	4:H:81:LEU:CD1	2.32	0.59
2:B:70:GLN:NE2	2:B:71:ARG:HD3	2.17	0.59
1:A:73:MSE:HE1	1:A:76:ARG:HD2	1.84	0.59
2:B:176:GLU:CG	2:B:183:PRO:HB3	2.33	0.59
5:K:23:LYS:HG2	5:K:72:SER:HB3	1.83	0.59
2:B:139:LYS:O	2:B:142:VAL:HG22	2.03	0.59
1:D:23:MSE:HE3	1:D:25:ASP:N	2.18	0.58
2:B:106:THR:OG1	2:B:114:LEU:HD12	2.03	0.58
2:E:70:GLN:HE22	2:E:71:ARG:HD3	1.68	0.58
6:L:45:LEU:CD1	6:L:59:ASP:H	2.16	0.58
5:K:101:PHE:CD2	6:L:43:LEU:HB2	2.38	0.58
1:D:92:LEU:HG	1:D:108:PHE:CE2	2.33	0.58
4:G:176:LEU:HA	7:G:223:HOH:O	2.04	0.58
4:G:164:ARG:O	4:G:168:GLY:HA3	2.03	0.58
6:J:9:ARG:CD	6:J:9:ARG:H	2.15	0.58
2:B:170:VAL:HG22	2:B:189:ARG:HE	1.69	0.58
2:B:51:THR:HG22	2:B:53:LEU:H	1.69	0.58
4:H:164:ARG:O	4:H:168:GLY:HA3	2.04	0.57
5:K:12:VAL:HG13	5:K:80:VAL:HG11	1.86	0.57
4:H:178:TRP:O	4:H:182:LEU:HD23	2.03	0.57
6:L:19:VAL:HB	6:L:78:LEU:HG	1.86	0.57
2:B:101:VAL:CG2	2:B:115:LEU:HD11	2.35	0.57
2:B:131:TRP:CE3	2:B:131:TRP:HA	2.40	0.57
2:E:118:SER:HA	2:E:158:LEU:HD22	1.86	0.57
4:G:60:PHE:O	4:G:63:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:70:LEU:N	4:H:70:LEU:HD12	2.18	0.57
1:A:92:LEU:HG	1:A:108:PHE:HE2	1.70	0.57
6:J:27:ASN:N	6:J:27:ASN:ND2	2.51	0.56
2:B:129:VAL:HB	2:B:159:VAL:HG21	1.87	0.56
2:E:172:THR:CG2	2:E:187:GLU:HG2	2.33	0.56
2:B:97:PRO:HB2	2:B:119:VAL:HG23	1.88	0.56
5:I:108:ILE:HD12	5:I:108:ILE:N	2.20	0.56
2:B:166:ARG:HG2	2:B:169:GLU:HG3	1.86	0.56
4:G:125:ASN:ND2	4:G:128:PHE:HB2	2.20	0.56
2:E:131:TRP:NE1	2:E:161:LEU:HB2	2.21	0.56
5:I:28:ALA:C	5:I:30:PRO:HD3	2.26	0.56
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.86	0.56
4:H:63:VAL:HG21	6:L:50:TYR:CD1	2.40	0.56
2:E:70:GLN:NE2	2:E:71:ARG:HD3	2.20	0.56
4:G:134:LYS:HZ1	4:G:170:ASP:CG	2.09	0.56
5:K:108:ILE:N	5:K:108:ILE:HD12	2.21	0.56
4:G:59:ALA:HB1	4:G:76:PHE:CE1	2.40	0.56
2:B:129:VAL:HG22	2:B:175:VAL:HG12	1.87	0.56
6:J:15:THR:HG22	6:J:111:SER:HB3	1.88	0.56
1:D:46:GLU:HG3	1:D:47:GLU:N	2.20	0.56
6:L:33:TYR:CE2	6:L:99:LEU:HD11	2.40	0.56
4:H:189:LEU:HD23	4:H:200:LEU:HD22	1.88	0.56
4:H:83:LEU:HD23	4:H:107:LEU:HD21	1.88	0.56
5:I:3:VAL:HG21	5:I:90:CYS:SG	2.46	0.56
6:J:76:LEU:HD23	6:J:77:ILE:N	2.20	0.56
4:H:63:VAL:HG23	4:H:72:TYR:CE1	2.41	0.56
5:K:28:ALA:C	5:K:30:PRO:HD3	2.27	0.56
5:K:46:LEU:HD12	5:K:47:LEU:HG	1.89	0.55
2:E:166:ARG:HG2	2:E:169:GLU:CG	2.35	0.55
4:G:51:LYS:NZ	4:G:108:ASP:OD1	2.32	0.55
4:G:106:ILE:O	4:G:110:ILE:HG13	2.07	0.55
2:B:132:PHE:HB2	2:B:172:THR:HG23	1.88	0.55
4:H:143:LYS:HD3	4:H:194:TYR:OH	2.06	0.55
4:G:188:TYR:CD2	6:J:96:GLY:HA3	2.41	0.55
4:G:176:LEU:HD13	4:G:178:TRP:NE1	2.21	0.55
4:H:17:GLN:O	4:H:73:LYS:HD3	2.07	0.55
5:K:91:ALA:HB2	5:K:101:PHE:HA	1.89	0.55
4:G:188:TYR:O	4:G:192:ARG:HD2	2.06	0.55
6:L:81:ALA:HA	6:L:85:GLN:HE21	1.71	0.55
5:I:26:TYR:CD1	5:I:28:ALA:HB3	2.42	0.55
2:E:129:VAL:HB	2:E:159:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MSE:HE2	2:B:53:LEU:HD13	1.89	0.55
5:I:21:ARG:HA	5:I:74:HIS:CD2	2.42	0.55
6:J:33:TYR:CD2	6:J:33:TYR:N	2.75	0.55
4:G:38:LYS:HB3	4:G:40:GLU:OE2	2.06	0.54
1:A:6:VAL:HG22	2:B:16:HIS:ND1	2.21	0.54
2:B:93:ARG:NH2	2:B:153:TRP:O	2.40	0.54
2:E:176:GLU:CG	2:E:183:PRO:HB3	2.37	0.54
4:G:153:LEU:HG	4:G:191:LYS:NZ	2.22	0.54
2:B:132:PHE:CE1	2:B:137:GLU:HB2	2.41	0.54
5:I:56:VAL:O	5:I:63:GLU:HG3	2.07	0.54
4:G:192:ARG:O	4:G:197:ASP:HB3	2.08	0.54
2:E:94:ARG:HG2	2:E:94:ARG:HH11	1.72	0.54
5:I:13:SER:HA	5:I:110:LEU:HB2	1.90	0.54
1:A:23:MSE:HE1	1:A:139:PRO:CD	2.37	0.54
6:J:99:LEU:N	6:J:99:LEU:HD22	2.23	0.54
6:L:81:ALA:HA	6:L:85:GLN:NE2	2.22	0.54
1:A:73:MSE:HE1	2:B:53:LEU:HD22	1.88	0.54
2:E:189:ARG:HG3	2:E:189:ARG:HH21	1.73	0.54
1:D:3:GLU:HA	2:E:18:PHE:CD2	2.43	0.54
1:D:23:MSE:HE3	1:D:24:PHE:C	2.28	0.54
4:H:70:LEU:H	4:H:70:LEU:CD1	2.19	0.54
1:D:122:LEU:HB2	1:D:162:ASP:HB2	1.89	0.54
5:K:3:VAL:HG23	5:K:22:CYS:SG	2.48	0.54
5:K:34:TRP:CD1	5:K:47:LEU:HD11	2.43	0.53
4:G:143:LYS:HE3	4:G:193:TYR:CE2	2.43	0.53
5:I:19:GLN:HA	5:I:75:LEU:O	2.07	0.53
1:D:129:THR:O	1:D:132:VAL:HG22	2.08	0.53
2:B:101:VAL:HG22	2:B:115:LEU:HD11	1.90	0.53
2:E:131:TRP:CD1	2:E:161:LEU:HB2	2.42	0.53
6:J:68:ARG:NH2	6:J:70:SER:O	2.42	0.53
2:E:102:TYR:O	2:E:116:VAL:HG22	2.09	0.53
5:K:19:GLN:HA	5:K:75:LEU:O	2.08	0.53
2:B:132:PHE:CB	2:B:172:THR:HG23	2.39	0.53
5:K:40:ARG:O	5:K:40:ARG:HG2	2.09	0.53
1:A:160:VAL:HG13	1:A:160:VAL:O	2.08	0.53
4:H:27:LYS:HE3	4:H:27:LYS:HA	1.90	0.53
4:H:44:VAL:HA	4:H:47:LEU:CD2	2.31	0.53
5:K:48:LYS:HE3	5:K:50:TYR:CE1	2.41	0.53
2:E:189:ARG:O	2:E:190:ALA:HB2	2.09	0.53
6:L:82:THR:H	6:L:85:GLN:HE21	1.55	0.53
2:B:127:ILE:CG1	2:B:177:HIS:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ARG:HG2	2:B:94:ARG:HH11	1.73	0.53
5:I:47:LEU:HD21	5:I:75:LEU:CD1	2.40	0.52
2:B:51:THR:HG22	2:B:53:LEU:N	2.24	0.52
1:A:103:ASN:HB3	1:A:153:PHE:CE1	2.44	0.52
4:H:193:TYR:CE1	4:H:198:ILE:HA	2.44	0.52
4:H:152:ASP:OD1	4:H:154:ARG:HG2	2.09	0.52
4:H:154:ARG:NH2	5:K:59:VAL:HG21	2.22	0.52
1:A:134:GLU:HG2	7:A:223:HOH:O	2.09	0.52
1:D:144:LEU:HD13	2:E:34:GLN:NE2	2.25	0.52
5:I:23:LYS:HG2	5:I:72:SER:HB3	1.92	0.52
4:H:63:VAL:HG23	4:H:72:TYR:HE1	1.74	0.52
4:H:142:MET:CE	4:H:167:PHE:HE1	2.23	0.52
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.43	0.52
4:H:160:ILE:CG2	6:L:28:ASN:HB3	2.39	0.52
2:B:70:GLN:HE22	2:B:71:ARG:HD3	1.74	0.52
2:E:106:THR:HG22	2:E:114:LEU:HB2	1.92	0.52
6:L:83:PRO:HA	6:L:109:VAL:HB	1.91	0.52
4:H:90:GLN:HE21	4:H:103:ASN:HD22	1.58	0.52
5:K:13:SER:HA	5:K:110:LEU:HB2	1.91	0.52
5:I:99:LEU:CG	6:J:99:LEU:HD23	2.37	0.52
4:G:192:ARG:HD3	5:I:50:TYR:CZ	2.45	0.52
2:E:138:GLU:HG2	2:E:161:LEU:HD11	1.90	0.52
4:G:16:VAL:HG21	4:G:81:LEU:CD1	2.37	0.52
4:H:16:VAL:HG22	4:H:19:LEU:HD12	1.92	0.52
6:L:66:ALA:HB1	6:L:74:PHE:CE2	2.45	0.52
6:L:9:ARG:NH2	6:L:103:ALA:HB1	2.25	0.51
2:B:129:VAL:HA	2:B:175:VAL:HG12	1.91	0.51
2:B:152:ASP:O	2:B:153:TRP:HB2	2.09	0.51
4:H:188:TYR:O	4:H:192:ARG:HG3	2.10	0.51
4:G:27:LYS:HA	4:G:27:LYS:HE3	1.91	0.51
5:I:3:VAL:CG2	5:I:90:CYS:SG	2.99	0.51
1:A:142:ASP:OD1	1:A:144:LEU:HB2	2.11	0.51
2:B:170:VAL:HG22	2:B:189:ARG:NE	2.26	0.51
2:B:129:VAL:CB	2:B:159:VAL:HG21	2.40	0.51
5:I:26:TYR:CE1	5:I:28:ALA:HB3	2.45	0.51
4:H:153:LEU:O	4:H:155:ASP:N	2.44	0.51
4:H:6:GLU:O	4:H:8:PRO:HD3	2.10	0.51
6:L:45:LEU:HD13	6:L:59:ASP:H	1.74	0.51
1:A:34:VAL:HG21	1:A:59:ALA:HB3	1.93	0.51
4:G:6:GLU:O	4:G:8:PRO:HD3	2.10	0.51
4:H:78:MET:O	4:H:82:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:167:PHE:O	4:G:169:SER:N	2.44	0.51
2:E:134:ASN:HB3	2:E:170:VAL:HB	1.92	0.51
6:L:64:TYR:CD1	6:L:78:LEU:HD22	2.43	0.51
5:K:47:LEU:O	5:K:47:LEU:HD12	2.11	0.51
4:G:159:ALA:O	4:G:163:VAL:HG23	2.11	0.51
1:A:97:VAL:O	1:A:98:GLU:HG3	2.11	0.50
1:A:129:THR:O	1:A:132:VAL:HG22	2.11	0.50
5:I:47:LEU:HD12	5:I:47:LEU:O	2.11	0.50
4:G:176:LEU:HD13	4:G:178:TRP:HE1	1.76	0.50
2:E:93:ARG:O	2:E:94:ARG:HG2	2.10	0.50
4:G:78:MET:O	4:G:82:LYS:HG3	2.11	0.50
1:A:99:LEU:HD11	1:A:180:PHE:CZ	2.46	0.50
4:G:144:ILE:C	4:G:146:LEU:H	2.14	0.50
2:B:143:VAL:CG1	2:B:160:MET:HB2	2.40	0.50
1:A:23:MSE:CE	1:A:138:LEU:HA	2.38	0.50
4:G:198:ILE:HG22	4:G:198:ILE:O	2.11	0.50
1:A:99:LEU:O	1:A:100:ARG:HB2	2.12	0.50
2:B:189:ARG:O	2:B:190:ALA:HB2	2.11	0.50
2:E:106:THR:CG2	2:E:114:LEU:HB2	2.41	0.50
4:G:142:MET:CE	4:G:187:VAL:HG12	2.42	0.50
2:B:133:ARG:HD2	2:B:136:GLN:OE1	2.11	0.50
6:J:15:THR:O	6:J:15:THR:HG23	2.11	0.50
1:D:124:ASN:OD1	1:D:160:VAL:HG12	2.12	0.50
5:K:55:VAL:HG23	5:K:55:VAL:O	2.11	0.50
4:H:154:ARG:HH11	4:H:154:ARG:HG2	1.75	0.50
2:E:133:ARG:HD2	2:E:136:GLN:OE1	2.12	0.50
2:E:148:ILE:HB	2:E:156:GLN:O	2.12	0.50
2:E:164:VAL:HG23	2:E:164:VAL:O	2.12	0.50
4:H:40:GLU:CD	4:H:40:GLU:H	2.14	0.50
6:J:68:ARG:HH22	6:J:71:GLN:HA	1.77	0.50
2:E:118:SER:HA	2:E:158:LEU:CD2	2.42	0.50
5:K:49:TYR:CE2	5:K:54:PRO:HA	2.46	0.49
4:G:142:MET:SD	4:G:167:PHE:HE1	2.34	0.49
2:B:122:PHE:CD1	2:B:127:ILE:HD12	2.47	0.49
5:I:89:PHE:CE1	5:I:104:GLY:HA3	2.48	0.49
1:A:15:ASN:ND2	1:A:70:LEU:HD13	2.28	0.49
1:A:99:LEU:HA	1:A:155:PRO:HB2	1.94	0.49
2:E:18:PHE:HB2	2:E:23:ARG:HB3	1.93	0.49
1:A:135:THR:HG23	1:A:136:VAL:O	2.12	0.49
2:E:94:ARG:HG2	2:E:94:ARG:NH1	2.28	0.49
4:H:144:ILE:C	4:H:146:LEU:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:59:VAL:HG12	5:K:60:ASN:N	2.28	0.49
2:E:36:GLU:HG2	2:E:50:VAL:HG21	1.94	0.49
4:G:89:THR:HG21	4:G:99:GLN:OE1	2.13	0.49
1:D:12:PHE:C	1:D:12:PHE:CD1	2.86	0.49
5:K:49:TYR:CE1	5:K:51:SER:HA	2.48	0.49
5:I:110:LEU:N	5:I:110:LEU:HD22	2.27	0.49
1:A:121:TRP:CE2	1:A:151:LEU:HB2	2.48	0.48
6:J:45:LEU:HD13	6:J:59:ASP:H	1.78	0.48
1:A:12:PHE:C	1:A:12:PHE:CD1	2.86	0.48
1:A:94:ASN:HB2	1:A:104:VAL:HB	1.95	0.48
4:H:160:ILE:CG2	6:L:28:ASN:CB	2.92	0.48
4:H:167:PHE:O	4:H:169:SER:N	2.47	0.48
1:A:99:LEU:HD12	1:A:99:LEU:N	2.14	0.48
2:B:148:ILE:HB	2:B:156:GLN:O	2.13	0.48
4:G:65:ASP:OD1	4:G:204:SER:HB2	2.13	0.48
1:A:117:VAL:HG23	1:A:166:GLU:O	2.13	0.48
4:G:153:LEU:HD13	5:I:48:LYS:HZ3	1.77	0.48
1:A:110:ASP:OD2	1:A:111:LYS:N	2.46	0.48
4:G:200:LEU:HA	4:G:203:THR:OG1	2.14	0.48
2:E:129:VAL:CB	2:E:159:VAL:HG21	2.44	0.48
2:B:51:THR:CG2	2:B:53:LEU:H	2.26	0.48
4:G:185:LYS:O	4:G:189:LEU:HG	2.13	0.47
3:F:318:THR:HG22	3:F:318:THR:O	2.14	0.47
4:G:153:LEU:C	4:G:155:ASP:H	2.15	0.47
2:E:176:GLU:HG2	2:E:183:PRO:HB3	1.96	0.47
1:A:113:THR:OG1	1:A:114:PRO:HA	2.14	0.47
4:G:47:LEU:N	4:G:47:LEU:HD22	2.30	0.47
2:E:189:ARG:CG	2:E:189:ARG:HH21	2.26	0.47
4:G:142:MET:HE1	4:G:187:VAL:HG12	1.95	0.47
4:H:159:ALA:O	4:H:163:VAL:HG23	2.15	0.47
5:K:38:TYR:O	5:K:41:GLN:HB2	2.13	0.47
1:D:89:VAL:O	1:D:176:LYS:NZ	2.46	0.47
1:D:92:LEU:C	1:D:92:LEU:HD12	2.35	0.47
4:H:149:GLN:HG2	4:H:162:LYS:NZ	2.30	0.47
4:G:97:VAL:HG23	4:G:98:GLU:N	2.30	0.47
4:G:154:ARG:HD3	4:G:154:ARG:N	2.06	0.47
6:J:111:SER:O	6:J:112:SER:HB2	2.14	0.47
6:J:36:ARG:O	6:J:36:ARG:HG3	2.15	0.47
5:K:34:TRP:HB2	5:K:47:LEU:CD1	2.45	0.47
2:E:62:ASN:HD22	2:E:68:LEU:HD11	1.79	0.47
4:H:193:TYR:CB	4:H:200:LEU:HD12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:99:LEU:HG	6:J:99:LEU:CD2	2.42	0.47
4:G:120:TYR:O	4:G:124:GLN:HG2	2.15	0.47
1:D:48:PHE:N	1:D:48:PHE:CD2	2.83	0.47
6:L:36:ARG:HH22	6:L:85:GLN:HA	1.78	0.46
1:D:118:ASN:HB3	1:D:166:GLU:HB2	1.97	0.46
5:K:49:TYR:CD1	5:K:49:TYR:C	2.89	0.46
6:J:15:THR:CG2	6:J:111:SER:HB3	2.45	0.46
5:I:101:PHE:HD2	6:J:43:LEU:HB2	1.79	0.46
4:H:142:MET:HG2	4:H:146:LEU:CD1	2.45	0.46
2:E:180:VAL:HG21	2:E:184:LEU:HD13	1.96	0.46
6:L:29:HIS:HB3	6:L:94:GLY:O	2.16	0.46
2:E:45:GLY:O	2:E:72:ARG:HD3	2.15	0.46
4:G:184:VAL:HG23	4:G:185:LYS:N	2.30	0.46
6:J:9:ARG:HD2	6:J:10:ASN:H	1.79	0.46
5:I:29:THR:N	5:I:30:PRO:HD3	2.30	0.46
5:K:10:VAL:HG11	5:K:18:LEU:HD11	1.96	0.46
6:L:15:THR:HG23	6:L:15:THR:O	2.16	0.46
2:B:106:THR:HG21	2:B:114:LEU:CD1	2.45	0.46
2:E:128:GLU:O	2:E:175:VAL:HA	2.16	0.46
4:G:131:LEU:HD22	4:G:179:PHE:CE2	2.51	0.46
2:B:171:TYR:O	2:B:188:TRP:N	2.47	0.46
4:H:113:LYS:HE3	4:H:117:ASP:OD1	2.16	0.46
1:A:180:PHE:O	1:A:181:ASP:HB3	2.16	0.46
2:E:166:ARG:O	2:E:169:GLU:HG3	2.15	0.46
4:G:192:ARG:HD3	5:I:50:TYR:CE2	2.50	0.46
2:E:21:THR:O	2:E:80:ARG:NH1	2.48	0.46
1:D:158:GLU:N	1:D:158:GLU:OE1	2.49	0.46
1:A:141:GLU:HG3	7:A:207:HOH:O	2.15	0.46
4:H:97:VAL:HG22	7:H:237:HOH:O	2.16	0.46
4:H:146:LEU:HA	4:H:149:GLN:HB2	1.97	0.46
5:I:55:VAL:HG23	5:I:55:VAL:O	2.16	0.46
6:J:83:PRO:HA	6:J:109:VAL:HB	1.98	0.46
4:H:51:LYS:HA	4:H:51:LYS:HD3	1.71	0.46
4:G:63:VAL:HG21	6:J:50:TYR:CD1	2.51	0.46
4:G:176:LEU:HB2	4:G:179:PHE:HB2	1.97	0.46
4:G:60:PHE:CA	4:G:63:VAL:HG12	2.45	0.46
2:E:171:TYR:O	2:E:188:TRP:N	2.48	0.46
1:D:141:GLU:HB3	7:E:223:HOH:O	2.16	0.46
5:I:12:VAL:CG1	5:I:80:VAL:HG11	2.46	0.46
4:H:154:ARG:HG2	4:H:154:ARG:NH1	2.31	0.45
4:H:40:GLU:N	4:H:40:GLU:OE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ASN:HB2	1:D:104:VAL:HB	1.98	0.45
1:A:77:SER:O	1:A:78:ASN:CB	2.64	0.45
6:L:33:TYR:N	6:L:33:TYR:CD2	2.83	0.45
1:D:37:ALA:HB1	4:H:99:GLN:NE2	2.31	0.45
5:K:60:ASN:O	5:K:77:LYS:HE3	2.16	0.45
1:D:98:GLU:O	1:D:101:GLU:HB2	2.16	0.45
5:I:34:TRP:CD1	5:I:47:LEU:HD11	2.52	0.45
2:B:174:GLN:HG2	2:B:175:VAL:N	2.31	0.45
4:G:170:ASP:O	4:G:174:LYS:HG3	2.15	0.45
4:H:153:LEU:O	4:H:154:ARG:C	2.55	0.45
2:E:28:GLU:OE2	2:E:71:ARG:NE	2.46	0.45
2:E:118:SER:CA	2:E:158:LEU:HD22	2.46	0.45
5:I:38:TYR:HB2	5:I:41:GLN:NE2	2.31	0.45
5:K:20:LEU:HD12	5:K:105:THR:HG21	1.98	0.45
3:C:318:THR:O	3:C:318:THR:HG22	2.16	0.45
4:H:160:ILE:HD12	6:L:27:ASN:O	2.16	0.45
5:I:36:VAL:HB	5:I:46:LEU:HD23	1.97	0.45
2:B:128:GLU:O	2:B:175:VAL:HA	2.16	0.45
4:H:6:GLU:C	4:H:8:PRO:HD3	2.37	0.45
1:D:45:LEU:HB2	1:D:48:PHE:CE2	2.52	0.45
1:D:92:LEU:HD11	1:D:108:PHE:HZ	1.82	0.45
4:H:134:LYS:HZ1	4:H:170:ASP:CG	2.19	0.45
1:D:45:LEU:HD12	7:D:244:HOH:O	2.16	0.45
5:I:6:PRO:HG2	5:I:7:ASP:OD1	2.17	0.45
6:J:78:LEU:HA	6:J:78:LEU:HD23	1.66	0.45
2:E:74:ALA:O	2:E:78:TYR:HB3	2.16	0.45
6:L:43:LEU:N	6:L:43:LEU:HD22	2.32	0.45
2:B:18:PHE:HB2	2:B:23:ARG:HB3	1.99	0.45
4:G:59:ALA:HA	4:G:79:MET:CE	2.44	0.44
2:E:103:PRO:HD3	2:E:188:TRP:CH2	2.52	0.44
1:D:175:LEU:HD12	1:D:175:LEU:N	2.32	0.44
2:B:166:ARG:NH1	2:B:169:GLU:HG2	2.33	0.44
2:B:41:ASP:HB3	2:B:44:VAL:HG23	2.00	0.44
4:G:17:GLN:CD	4:G:17:GLN:H	2.21	0.44
4:G:140:LYS:NZ	4:G:210:VAL:O	2.49	0.44
6:J:81:ALA:HA	6:J:85:GLN:HE22	1.82	0.44
5:I:91:ALA:HB2	5:I:101:PHE:CD1	2.53	0.44
6:J:43:LEU:HD22	6:J:43:LEU:N	2.32	0.44
4:G:188:TYR:CE2	6:J:96:GLY:HA3	2.53	0.44
4:G:184:VAL:O	4:G:188:TYR:HD1	2.00	0.44
2:B:113:ASN:HB2	2:B:163:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:VAL:HG12	2:B:186:VAL:HG12	1.99	0.44
5:K:16:ALA:O	5:K:80:VAL:HG23	2.17	0.44
6:L:40:GLY:C	6:L:41:HIS:ND1	2.70	0.44
1:A:126:LYS:HA	1:A:127:PRO:HD3	1.90	0.44
5:K:40:ARG:O	5:K:40:ARG:CG	2.65	0.44
1:D:92:LEU:O	1:D:92:LEU:HD12	2.18	0.44
6:J:88:VAL:HA	6:J:105:THR:O	2.18	0.44
2:B:116:VAL:CG1	2:B:160:MET:HG2	2.29	0.44
2:E:101:VAL:HG12	2:E:186:VAL:HG12	1.99	0.44
1:A:39:LYS:CE	1:A:60:LEU:HD13	2.48	0.44
2:B:106:THR:HG21	2:B:114:LEU:HD12	1.99	0.44
1:D:106:ILE:HG12	1:D:150:TYR:HD1	1.83	0.44
2:B:100:THR:O	2:B:117:CYS:O	2.35	0.44
4:G:142:MET:O	4:G:146:LEU:HD12	2.17	0.44
2:E:51:THR:CG2	2:E:53:LEU:H	2.31	0.44
4:H:192:ARG:O	4:H:197:ASP:HB3	2.18	0.44
4:G:102:ARG:O	4:G:106:ILE:HG13	2.17	0.44
5:I:82:ARG:HA	5:I:109:VAL:HG11	1.99	0.44
5:K:29:THR:N	5:K:30:PRO:HD3	2.33	0.44
4:G:78:MET:HG3	7:G:219:HOH:O	2.18	0.44
6:L:25:GLN:HE22	6:L:29:HIS:H	1.64	0.44
5:I:53:ASP:OD2	5:I:55:VAL:HG22	2.18	0.44
1:D:113:THR:OG1	1:D:114:PRO:HA	2.18	0.44
6:J:86:THR:HG23	6:J:108:SER:HA	2.00	0.44
1:A:82:ILE:HB	2:B:33:ASN:OD1	2.16	0.44
2:B:164:VAL:HG23	2:B:164:VAL:O	2.18	0.44
4:G:199:GLU:HG3	5:I:51:SER:HB3	2.00	0.44
4:G:47:LEU:H	4:G:47:LEU:HD22	1.82	0.43
2:B:129:VAL:HG11	2:B:159:VAL:HG21	1.99	0.43
4:H:162:LYS:HD3	4:H:165:GLU:OE1	2.18	0.43
5:I:32:LEU:HD23	5:I:92:VAL:HG12	2.00	0.43
5:K:18:LEU:O	5:K:76:ARG:HA	2.19	0.43
4:G:52:VAL:O	4:G:55:PHE:HB3	2.18	0.43
4:H:192:ARG:HB2	4:H:200:LEU:HD11	2.01	0.43
5:I:34:TRP:HB2	5:I:47:LEU:CD1	2.49	0.43
2:E:129:VAL:HG11	2:E:159:VAL:HG21	2.00	0.43
5:I:23:LYS:HG2	5:I:72:SER:CB	2.47	0.43
6:L:78:LEU:N	6:L:78:LEU:HD23	2.33	0.43
2:E:133:ARG:HE	2:E:171:TYR:HE1	1.65	0.43
1:D:109:ILE:HD12	1:D:165:VAL:HG21	2.00	0.43
4:G:136:VAL:HG13	4:G:210:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:HA	1:A:50:ARG:HD2	2.01	0.43
2:B:143:VAL:HG13	2:B:160:MET:HB2	2.01	0.43
2:B:131:TRP:CG	2:B:161:LEU:HD22	2.53	0.43
6:J:68:ARG:HH22	6:J:71:GLN:CA	2.32	0.43
2:B:129:VAL:CG1	2:B:159:VAL:HG21	2.49	0.43
5:K:110:LEU:HD22	5:K:110:LEU:N	2.34	0.43
3:C:315:LYS:HG2	3:C:316:LEU:O	2.19	0.43
4:H:21:ASN:HD22	6:L:56:GLU:HA	1.83	0.43
4:H:4:ARG:HD2	4:H:205:ASP:OD2	2.19	0.43
1:A:92:LEU:HG	1:A:108:PHE:CE2	2.53	0.43
2:E:10:GLN:HB2	2:E:31:ILE:HB	2.00	0.43
4:H:160:ILE:HG21	6:L:28:ASN:HB3	1.99	0.43
2:B:55:ARG:HB2	2:B:56:PRO:HD3	2.01	0.43
2:E:157:THR:O	2:E:158:LEU:HD23	2.18	0.43
1:A:109:ILE:HD12	1:A:165:VAL:HG21	2.01	0.43
5:I:67:SER:O	5:I:71:SER:N	2.52	0.43
2:E:51:THR:HG23	2:E:53:LEU:H	1.82	0.43
4:G:40:GLU:OE2	4:G:40:GLU:N	2.36	0.43
5:K:33:PHE:HE1	5:K:93:SER:HB2	1.84	0.43
5:I:5:GLN:OE1	5:I:104:GLY:N	2.48	0.42
5:I:12:VAL:HG13	5:I:80:VAL:HG11	2.01	0.42
5:I:16:ALA:O	5:I:80:VAL:HG23	2.19	0.42
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.53	0.42
1:D:100:ARG:HA	1:D:154:LEU:HD11	1.99	0.42
6:J:76:LEU:C	6:J:76:LEU:HD23	2.40	0.42
2:E:129:VAL:CG1	2:E:159:VAL:HG21	2.50	0.42
2:E:100:THR:O	2:E:117:CYS:O	2.37	0.42
2:E:75:VAL:O	2:E:79:CYS:HB2	2.19	0.42
4:H:126:LYS:O	4:H:130:GLU:HG3	2.18	0.42
4:H:181:SER:O	4:H:184:VAL:HG22	2.19	0.42
2:E:27:LEU:HA	2:E:27:LEU:HD23	1.87	0.42
1:D:135:THR:HG23	1:D:136:VAL:N	2.35	0.42
6:L:87:SER:OG	6:L:88:VAL:N	2.52	0.42
4:G:211:PHE:CD2	4:G:211:PHE:N	2.85	0.42
5:I:18:LEU:O	5:I:76:ARG:HA	2.20	0.42
4:H:142:MET:HE3	4:H:167:PHE:HE1	1.84	0.42
5:K:36:VAL:CG1	5:K:46:LEU:HD23	2.49	0.42
5:I:13:SER:N	5:I:110:LEU:HD23	2.35	0.42
6:L:48:TYR:CZ	6:L:56:GLU:HB2	2.54	0.42
6:J:1:GLU:HG2	6:J:2:ALA:N	2.35	0.42
4:H:146:LEU:HD12	4:H:190:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:20:LEU:HD22	5:I:20:LEU:N	2.34	0.42
5:K:47:LEU:HD21	5:K:75:LEU:CD1	2.49	0.42
4:G:200:LEU:O	4:G:207:ALA:HB1	2.19	0.42
6:L:88:VAL:HA	6:L:105:THR:O	2.19	0.42
4:G:66:TYR:C	4:G:68:GLY:N	2.72	0.42
5:I:3:VAL:HA	5:I:24:TYR:HA	2.02	0.42
5:K:18:LEU:HD12	5:K:19:GLN:H	1.84	0.42
4:H:16:VAL:HG22	4:H:19:LEU:CD1	2.48	0.42
4:G:193:TYR:CB	4:G:200:LEU:HD12	2.50	0.42
5:I:49:TYR:C	5:I:49:TYR:CD1	2.93	0.42
1:D:135:THR:CG2	1:D:136:VAL:N	2.82	0.42
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.79	0.42
4:H:184:VAL:HG23	4:H:185:LYS:N	2.33	0.42
1:A:11:GLU:OE1	1:A:66:ASP:OD1	2.37	0.42
1:D:25:ASP:OD2	1:D:26:PHE:N	2.53	0.42
1:A:144:LEU:CD1	2:B:34:GLN:NE2	2.79	0.42
2:E:70:GLN:NE2	2:E:71:ARG:HH21	2.18	0.42
1:D:47:GLU:H	1:D:47:GLU:HG3	1.59	0.42
4:H:83:LEU:HD23	4:H:107:LEU:CD2	2.49	0.42
4:H:171:LYS:N	4:H:171:LYS:HD2	2.34	0.42
6:J:48:TYR:CZ	6:J:56:GLU:HB2	2.55	0.42
1:D:39:LYS:CE	1:D:60:LEU:HD13	2.47	0.42
4:G:178:TRP:O	4:G:182:LEU:HD23	2.20	0.42
4:H:65:ASP:OD1	4:H:204:SER:HB2	2.20	0.42
4:G:41:THR:O	4:G:44:VAL:HG12	2.19	0.41
5:K:59:VAL:O	5:K:60:ASN:HB3	2.20	0.41
5:K:32:LEU:HB3	5:K:73:PHE:CD2	2.55	0.41
4:G:186:GLY:O	4:G:190:ILE:HD13	2.20	0.41
2:B:101:VAL:HG22	2:B:102:TYR:N	2.34	0.41
2:E:174:GLN:HG2	2:E:175:VAL:N	2.35	0.41
4:H:192:ARG:HH11	4:H:200:LEU:HD21	1.84	0.41
1:A:73:MSE:HE3	1:A:76:ARG:HB3	2.02	0.41
1:D:106:ILE:HG12	1:D:150:TYR:CD1	2.55	0.41
6:L:51:GLY:O	6:L:68:ARG:HG2	2.21	0.41
6:J:78:LEU:HD22	6:J:85:GLN:OE1	2.21	0.41
4:H:41:THR:O	4:H:44:VAL:HG12	2.20	0.41
6:J:68:ARG:HH22	6:J:71:GLN:C	2.23	0.41
1:A:3:GLU:HA	2:B:18:PHE:CE2	2.56	0.41
4:G:51:LYS:CG	4:G:104:ILE:HG23	2.37	0.41
2:E:163:THR:OG1	2:E:165:PRO:HD3	2.20	0.41
2:B:129:VAL:HG22	2:B:175:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:46:LEU:HD13	5:K:46:LEU:O	2.20	0.41
2:B:157:THR:O	2:B:158:LEU:HD23	2.20	0.41
2:E:101:VAL:CG2	2:E:102:TYR:N	2.84	0.41
1:D:8:ILE:HB	1:D:25:ASP:HB3	2.03	0.41
5:I:60:ASN:O	5:I:77:LYS:HE3	2.20	0.41
4:G:66:TYR:C	4:G:68:GLY:H	2.24	0.41
4:G:71:GLU:HG2	4:G:121:PHE:CD2	2.56	0.41
1:A:13:TYR:OH	4:G:88:ASP:OD2	2.28	0.41
2:E:101:VAL:HG12	2:E:186:VAL:CG1	2.51	0.41
4:H:188:TYR:CD2	6:L:96:GLY:HA3	2.56	0.41
5:I:47:LEU:HD12	5:I:47:LEU:C	2.41	0.41
1:D:164:ARG:HH12	1:D:166:GLU:CD	2.23	0.41
2:B:75:VAL:O	2:B:79:CYS:HB2	2.20	0.41
2:B:102:TYR:CZ	2:B:116:VAL:HG21	2.55	0.41
6:J:36:ARG:HH22	6:J:85:GLN:HA	1.84	0.41
1:D:92:LEU:HD11	1:D:108:PHE:CZ	2.55	0.41
4:G:198:ILE:CG2	4:G:198:ILE:O	2.69	0.41
1:D:45:LEU:HD21	2:E:153:TRP:CD1	2.56	0.41
5:I:49:TYR:CZ	5:I:51:SER:HA	2.56	0.41
1:D:20:GLY:H	1:D:36:MSE:SE	2.53	0.41
5:K:42:GLY:HA2	6:L:90:PHE:CE2	2.56	0.41
4:G:43:GLU:O	4:G:47:LEU:CD2	2.69	0.41
2:E:101:VAL:HG22	2:E:102:TYR:N	2.35	0.41
4:H:200:LEU:O	4:H:207:ALA:HB1	2.21	0.41
5:K:82:ARG:HA	5:K:109:VAL:HG11	2.02	0.41
5:K:67:SER:O	5:K:71:SER:N	2.54	0.41
4:G:177:TRP:CZ2	6:J:71:GLN:HB3	2.56	0.40
2:B:94:ARG:NH1	2:B:94:ARG:HG2	2.36	0.40
5:I:23:LYS:HA	5:I:72:SER:HA	2.02	0.40
2:E:116:VAL:HG23	2:E:116:VAL:O	2.20	0.40
1:A:39:LYS:HE3	1:A:60:LEU:HD13	2.03	0.40
4:G:139:THR:O	4:G:142:MET:HB2	2.21	0.40
1:A:118:ASN:HB3	1:A:166:GLU:HB2	2.04	0.40
4:H:66:TYR:C	4:H:68:GLY:N	2.74	0.40
6:J:20:THR:C	6:J:21:LEU:HD23	2.42	0.40
2:B:127:ILE:HG13	2:B:177:HIS:CB	2.48	0.40
5:I:20:LEU:N	5:I:75:LEU:O	2.51	0.40
5:K:34:TRP:HB2	5:K:47:LEU:HD12	2.03	0.40
4:G:144:ILE:O	4:G:146:LEU:N	2.55	0.40
4:G:10:LYS:HA	4:G:120:TYR:CE1	2.56	0.40
2:E:90:THR:HG22	2:E:153:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:55:ARG:HB2	2:E:56:PRO:HD3	2.03	0.40
4:H:52:VAL:O	4:H:55:PHE:HB3	2.21	0.40
1:D:154:LEU:HD13	1:D:155:PRO:HD2	2.03	0.40
5:K:48:LYS:CE	5:K:50:TYR:HE1	2.29	0.40
4:G:192:ARG:NH2	6:J:97:GLY:N	2.63	0.40
5:I:24:TYR:CE2	5:I:32:LEU:HD11	2.57	0.40
5:K:23:LYS:HA	5:K:72:SER:HA	2.02	0.40
5:I:110:LEU:HD22	5:I:110:LEU:H	1.85	0.40
2:B:27:LEU:HD13	2:B:29:ARG:HD2	2.04	0.40
4:H:59:ALA:HA	4:H:79:MET:CE	2.52	0.40
4:G:63:VAL:HG13	4:G:64:ASN:N	2.36	0.40
2:B:37:SER:HA	2:B:51:THR:HB	2.04	0.40
2:B:166:ARG:O	2:B:169:GLU:HG3	2.22	0.40
4:G:82:LYS:NZ	7:G:244:HOH:O	2.38	0.40
1:D:82:ILE:HG13	2:E:33:ASN:HB3	2.04	0.40
1:D:87:PRO:CA	1:D:112:PHE:HB3	2.51	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	177/179 (99%)	168 (95%)	9 (5%)	0	100 100
1	D	177/179 (99%)	169 (96%)	8 (4%)	0	100 100
2	B	180/190 (95%)	167 (93%)	10 (6%)	3 (2%)	11 14
2	E	181/190 (95%)	169 (93%)	12 (7%)	0	100 100
3	C	11/13 (85%)	11 (100%)	0	0	100 100
3	F	11/13 (85%)	11 (100%)	0	0	100 100
4	G	211/213 (99%)	194 (92%)	14 (7%)	3 (1%)	14 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	H	211/213 (99%)	196 (93%)	12 (6%)	3 (1%)	14 18
5	I	109/110 (99%)	91 (84%)	12 (11%)	6 (6%)	2 1
5	K	107/110 (97%)	88 (82%)	14 (13%)	5 (5%)	3 1
6	J	111/113 (98%)	104 (94%)	3 (3%)	4 (4%)	4 3
6	L	109/113 (96%)	102 (94%)	3 (3%)	4 (4%)	4 3
All	All	1595/1636 (98%)	1470 (92%)	97 (6%)	28 (2%)	11 12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	154	ARG
4	H	154	ARG
6	J	97	GLY
6	L	97	GLY
4	G	145	LYS
4	G	168	GLY
4	H	145	LYS
4	H	168	GLY
5	I	14	GLU
5	K	14	GLU
6	J	95	GLY
5	K	27	SER
6	L	95	GLY
6	L	112	SER
5	I	16	ALA
5	I	27	SER
5	I	39	PRO
6	J	111	SER
6	J	112	SER
5	K	16	ALA
5	K	69	SER
2	B	134	ASN
5	I	51	SER
5	K	39	PRO
6	L	111	SER
2	B	118	SER
5	I	69	SER
2	B	178	PRO

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	164/161 (102%)	152 (93%)	12 (7%)	17 27
1	D	164/161 (102%)	152 (93%)	12 (7%)	17 27
2	B	165/171 (96%)	155 (94%)	10 (6%)	23 35
2	E	166/171 (97%)	154 (93%)	12 (7%)	18 27
3	C	12/12 (100%)	10 (83%)	2 (17%)	3 3
3	F	12/12 (100%)	10 (83%)	2 (17%)	3 3
4	G	196/196 (100%)	186 (95%)	10 (5%)	29 46
4	H	196/196 (100%)	187 (95%)	9 (5%)	33 50
5	I	94/93 (101%)	90 (96%)	4 (4%)	35 54
5	K	92/93 (99%)	88 (96%)	4 (4%)	35 54
6	J	92/92 (100%)	82 (89%)	10 (11%)	8 10
6	L	91/92 (99%)	81 (89%)	10 (11%)	8 10
All	All	1444/1450 (100%)	1347 (93%)	97 (7%)	20 31

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MSE
1	A	34	VAL
1	A	45	LEU
1	A	46	GLU
1	A	47	GLU
1	A	55	GLU
1	A	70	LEU
1	A	78	ASN
1	A	100	ARG
1	A	105	LEU
1	A	135	THR
1	A	144	LEU
2	B	11	LEU
2	B	23	ARG

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Mol	Chain	Res	Type
2	B	27	LEU
2	B	29	ARG
2	B	34	GLN
2	B	38	VAL
2	B	51	THR
2	B	68	LEU
2	B	70	GLN
2	B	131	TRP
3	C	307	LYS
3	C	310	LYS
1	D	17	ASP
1	D	23	MSE
1	D	44	ARG
1	D	46	GLU
1	D	47	GLU
1	D	70	LEU
1	D	99	LEU
1	D	135	THR
1	D	144	LEU
1	D	151	LEU
1	D	154	LEU
1	D	177	HIS
2	E	11	LEU
2	E	27	LEU
2	E	29	ARG
2	E	39	ARG
2	E	51	THR
2	E	68	LEU
2	E	70	GLN
2	E	94	ARG
2	E	113	ASN
2	E	114	LEU
2	E	119	VAL
2	E	131	TRP
3	F	307	LYS
3	F	310	LYS
4	G	27	LYS
4	G	45	LEU
4	G	72	TYR
4	G	116	ASN
4	G	149	GLN
4	G	154	ARG

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Mol	Chain	Res	Type
4	G	183	LEU
4	G	187	VAL
4	G	193	TYR
4	G	194	TYR
4	H	16	VAL
4	H	27	LYS
4	H	30	GLU
4	H	45	LEU
4	H	72	TYR
4	H	149	GLN
4	H	160	ILE
4	H	167	PHE
4	H	183	LEU
5	I	1	GLN
5	I	50	TYR
5	I	82	ARG
5	I	93	SER
6	J	9	ARG
6	J	25	GLN
6	J	27	ASN
6	J	28	ASN
6	J	33	TYR
6	J	36	ARG
6	J	42	GLU
6	J	45	LEU
6	J	62	ASP
6	J	79	GLU
5	K	9	ARG
5	K	19	GLN
5	K	31	TYR
5	K	50	TYR
6	L	25	GLN
6	L	28	ASN
6	L	36	ARG
6	L	42	GLU
6	L	45	LEU
6	L	62	ASP
6	L	76	LEU
6	L	78	LEU
6	L	79	GLU
6	L	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	B	62	ASN
2	B	92	GLN
1	D	118	ASN
2	E	10	GLN
2	E	34	GLN
2	E	62	ASN
2	E	70	GLN
2	E	107	GLN
2	E	113	ASN
4	G	21	ASN
4	G	34	ASN
4	G	64	ASN
4	G	77	ASN
4	G	90	GLN
4	G	103	ASN
4	G	116	ASN
4	G	129	GLN
4	G	161	ASN
4	H	20	ASN
4	H	21	ASN
4	H	34	ASN
4	H	64	ASN
4	H	77	ASN
4	H	90	GLN
4	H	99	GLN
4	H	161	ASN
5	I	1	GLN
5	I	19	GLN
5	I	41	GLN
5	I	44	GLN
5	I	60	ASN
5	I	81	HIS
6	J	25	GLN
6	J	27	ASN
6	J	30	ASN
6	J	85	GLN
5	K	19	GLN
5	K	41	GLN
5	K	57	GLN
5	K	60	ASN
6	L	24	ASN

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Mol	Chain	Res	Type
6	L	25	GLN
6	L	27	ASN
6	L	85	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	176/179 (98%)	-0.18	1 (0%) 90 90	22, 44, 73, 88	0
1	D	176/179 (98%)	-0.05	4 (2%) 64 63	25, 44, 74, 87	0
2	B	184/190 (96%)	0.56	27 (14%) 3 3	25, 54, 107, 112	0
2	E	185/190 (97%)	0.27	17 (9%) 11 10	26, 52, 106, 112	0
3	C	13/13 (100%)	0.04	0 100 100	35, 40, 52, 55	0
3	F	13/13 (100%)	-0.30	0 100 100	33, 38, 48, 54	0
4	G	213/213 (100%)	0.47	25 (11%) 6 6	33, 59, 102, 110	0
4	H	213/213 (100%)	0.03	6 (2%) 56 55	32, 55, 99, 108	0
5	I	110/110 (100%)	1.52	29 (26%) 1 1	69, 108, 118, 121	0
5	K	109/110 (99%)	1.54	31 (28%) 1 1	65, 107, 117, 119	0
6	J	113/113 (100%)	0.28	5 (4%) 38 38	41, 58, 80, 103	0
6	L	111/113 (98%)	0.23	4 (3%) 46 46	40, 56, 79, 102	0
All	All	1616/1636 (98%)	0.38	149 (9%) 11 10	22, 57, 110, 121	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	K	12	VAL	7.4
6	J	112	SER	7.3
5	I	80	VAL	6.5
5	I	110	LEU	6.4
5	I	26	TYR	6.2
4	G	1	MET	6.0
4	G	196	GLY	6.0
5	K	56	VAL	5.9
5	I	109	VAL	5.7
5	K	28	ALA	5.6
2	B	165	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	188	TRP	5.3
5	K	108	ILE	5.2
5	K	78	ALA	5.2
5	I	18	LEU	5.2
4	G	144	ILE	5.2
5	I	10	VAL	5.1
2	E	134	ASN	5.0
2	E	190	ALA	5.0
5	I	108	ILE	5.0
5	K	27	SER	4.8
5	K	80	VAL	4.8
5	K	10	VAL	4.7
4	G	150	LYS	4.6
4	G	189	LEU	4.6
2	E	132	PHE	4.6
4	G	149	GLN	4.6
5	K	11	THR	4.6
2	B	170	VAL	4.4
2	B	186	VAL	4.3
5	I	59	VAL	4.3
2	B	164	VAL	4.3
2	B	132	PHE	4.2
5	I	95[A]	PHE	4.2
2	B	134	ASN	4.1
2	E	115	LEU	4.0
5	K	104	GLY	4.0
6	J	113	ALA	3.9
2	B	114	LEU	3.9
4	G	194	TYR	3.9
6	L	112	SER	3.8
4	G	151	LEU	3.8
4	G	186	GLY	3.8
5	K	47	LEU	3.8
4	G	190	ILE	3.8
4	H	150	LYS	3.8
2	B	181	THR	3.7
2	E	106	THR	3.7
5	I	77	LYS	3.7
2	B	163	THR	3.7
6	L	113	ALA	3.7
2	B	141	GLY	3.6
2	B	190	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
4	H	153	LEU	3.6
5	K	50	TYR	3.6
5	I	75	LEU	3.5
5	K	18	LEU	3.5
4	G	198	ILE	3.5
2	B	189	ARG	3.4
2	B	133	ARG	3.4
2	B	140	ALA	3.4
2	B	105	LYS	3.4
5	K	79	SER	3.4
6	J	95	GLY	3.4
5	K	109	VAL	3.2
2	B	175	VAL	3.2
6	L	95	GLY	3.2
5	K	54	PRO	3.2
2	B	1	GLY	3.2
2	E	105	LYS	3.1
5	I	104	GLY	3.1
5	K	105	THR	3.1
2	B	167	SER	3.1
4	G	201	LYS	3.1
5	K	26	TYR	3.1
2	E	136	GLN	3.1
2	E	114	LEU	3.0
2	E	166	ARG	3.0
5	K	13	SER	3.0
2	E	170	VAL	3.0
4	G	136	VAL	2.9
5	I	55	VAL	2.9
4	G	192	ARG	2.9
2	E	162	GLU	2.9
5	K	3	VAL	2.9
1	D	100	ARG	2.9
1	D	108	PHE	2.9
5	I	81	HIS	2.9
5	I	17	SER	2.9
5	I	79	SER	2.8
5	I	56	VAL	2.8
2	B	131	TRP	2.7
5	I	24	TYR	2.7
4	H	149	GLN	2.7
2	B	171	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
4	G	200	LEU	2.7
5	K	57	GLN	2.7
6	J	111	SER	2.7
4	G	162	LYS	2.7
4	G	171	LYS	2.7
5	I	105	THR	2.6
2	E	164	VAL	2.6
2	B	130	ARG	2.6
4	G	153	LEU	2.6
5	K	76	ARG	2.5
4	G	147	LYS	2.5
5	I	76	ARG	2.5
2	E	167	SER	2.5
4	G	158	VAL	2.5
4	G	138	LEU	2.5
4	H	213	ASP	2.5
5	K	9	ARG	2.5
1	D	99	LEU	2.4
5	I	57	GLN	2.4
6	J	45	LEU	2.4
4	G	154	ARG	2.4
5	I	9	ARG	2.4
5	K	77	LYS	2.4
5	K	110	LEU	2.4
4	G	143	LYS	2.3
2	B	113	ASN	2.3
5	I	13	SER	2.3
2	B	183	PRO	2.3
5	I	78	ALA	2.3
5	I	31	TYR	2.3
5	K	81	HIS	2.3
4	H	200	LEU	2.2
5	K	7	ASP	2.2
5	I	14	GLU	2.2
5	I	27	SER	2.2
5	I	82	ARG	2.2
5	K	55	VAL	2.2
4	G	164	ARG	2.2
4	G	193	TYR	2.2
1	A	158	GLU	2.2
5	K	2	SER	2.2
2	E	1	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	104	SER	2.1
6	L	94	GLY	2.1
1	D	181	ASP	2.1
5	K	20	LEU	2.1
2	B	106	THR	2.1
2	E	184	LEU	2.1
2	B	173	CYS	2.1
2	E	175	VAL	2.1
2	B	172	THR	2.1
5	K	52	GLY	2.1
4	H	137	LYS	2.1
5	I	23	LYS	2.0

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

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

6.3 Carbohydrates

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.