Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:36 PM GMT

PDB ID	:	4R7N
Title	:	Fab C2E3
Authors	:	Loyau, J.; Didelot, G.; Malinge, P.; Ravn, U.; Magistrelli, G.; Depoisier, J.F.; Kosco-Vilbois, M.; Fischer, N.; Thore, S.; Rousseau, F.
Deposited on	:	2014-08-28
Resolution	:	3.45 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:

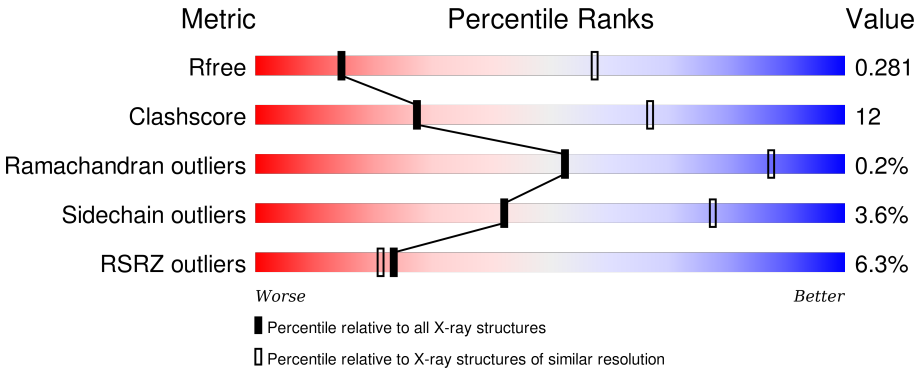
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	225	% 69% 25%
1	C	225	3% 74% 20%
1	E	225	6% 69% 26%
1	G	225	% 75% 20%
1	I	225	4% 76% 20%

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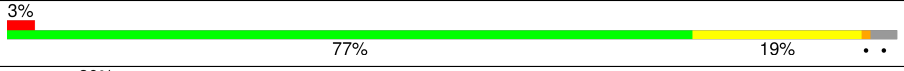
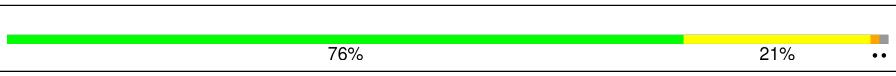
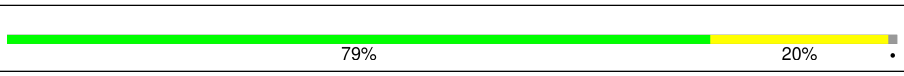
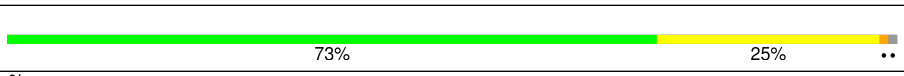
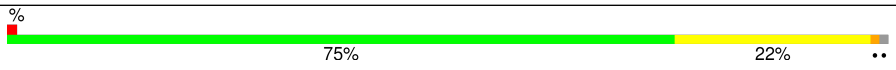
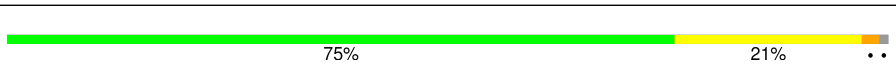
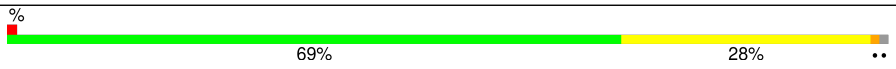
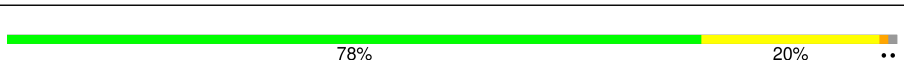
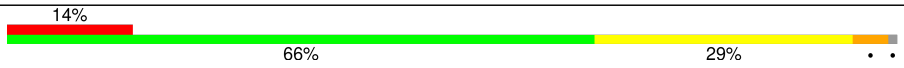
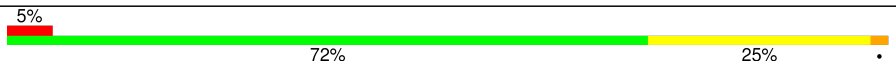
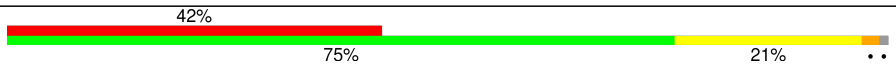
Mol	Chain	Length	Quality of chain
1	K	225	
1	M	225	
1	O	225	
1	Q	225	
1	S	225	
2	B	214	
2	D	214	
2	F	214	
2	H	214	
2	J	214	
2	L	214	
2	N	214	
2	P	214	
2	R	214	
2	T	214	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32933 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 Fab C2E3 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	C	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	E	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	G	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	I	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	K	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	M	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	O	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	Q	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			
1	S	218	Total	C	N	O	S	0	0	0
			1657	1056	276	320	5			

- Molecule 2 is a protein called Fab C2E3 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	D	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	F	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	H	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			

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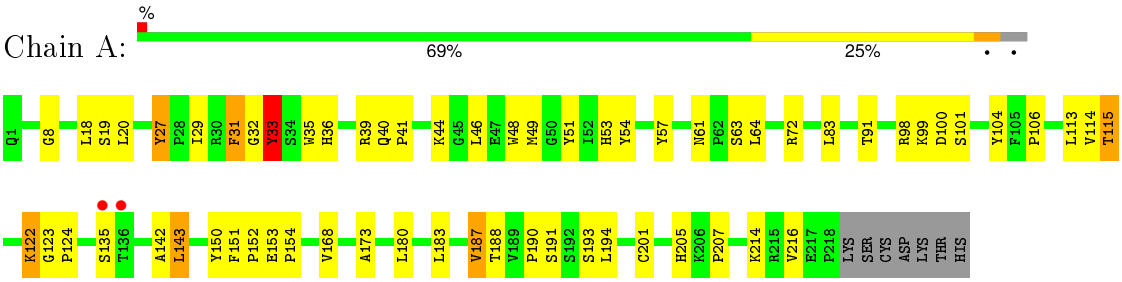
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	L	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	N	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	P	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	R	213	Total	C	N	O	S	0	0	0
			1648	1034	275	335	4			
2	T	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			

3 Residue-property plots (i)

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.

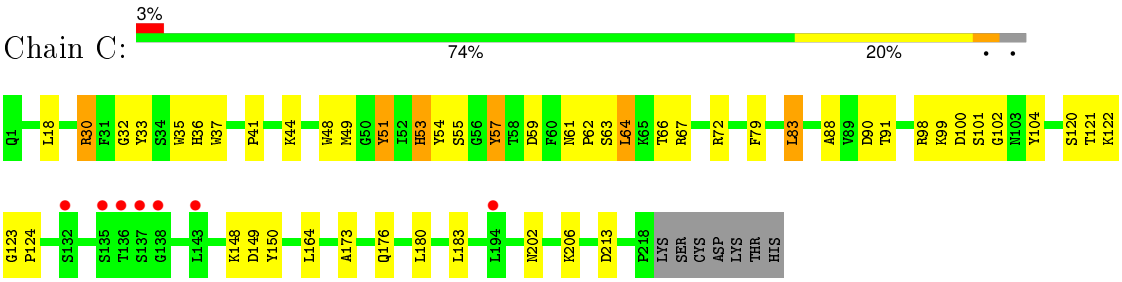
- Molecule 1: Fab C2E3 Heavy chain

Chain A:



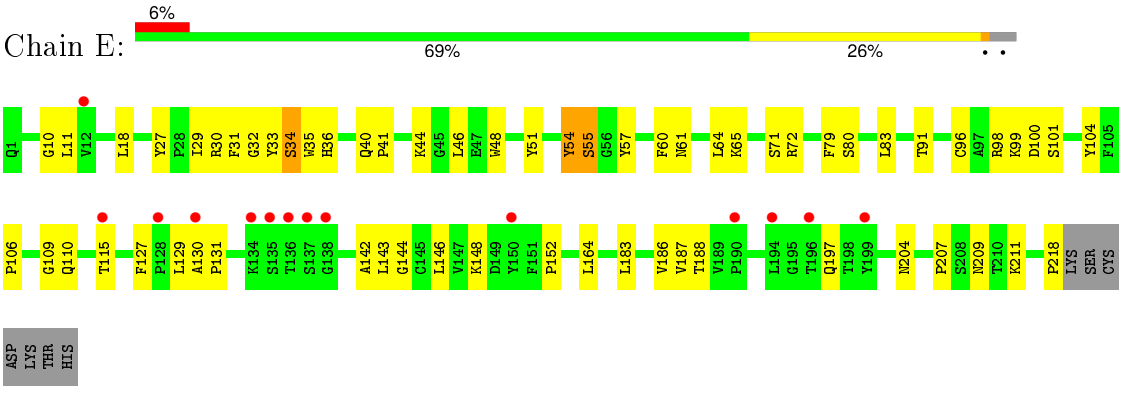
- Molecule 1: Fab C2E3 Heavy chain

Chain C:



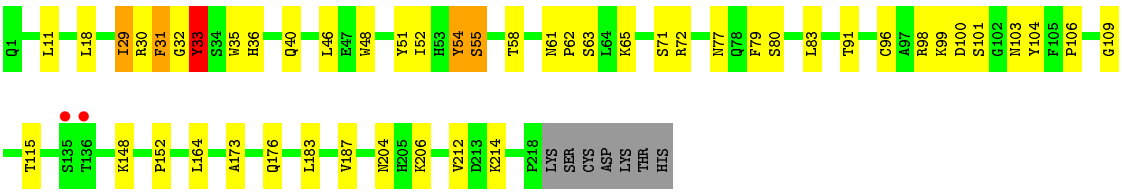
- Molecule 1: Fab C2E3 Heavy chain

Chain E:



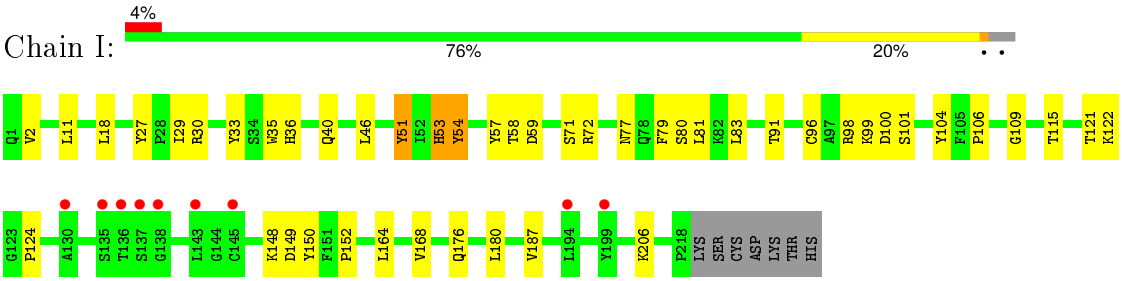
- Molecule 1: Fab C2E3 Heavy chain

Chain G:



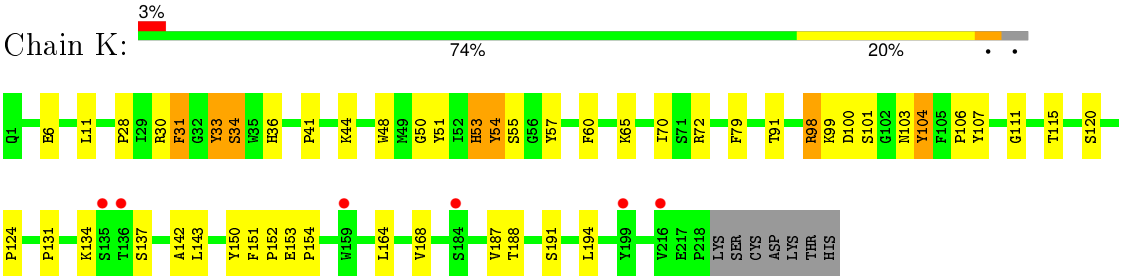
• Molecule 1: Fab C2E3 Heavy chain

Chain I:



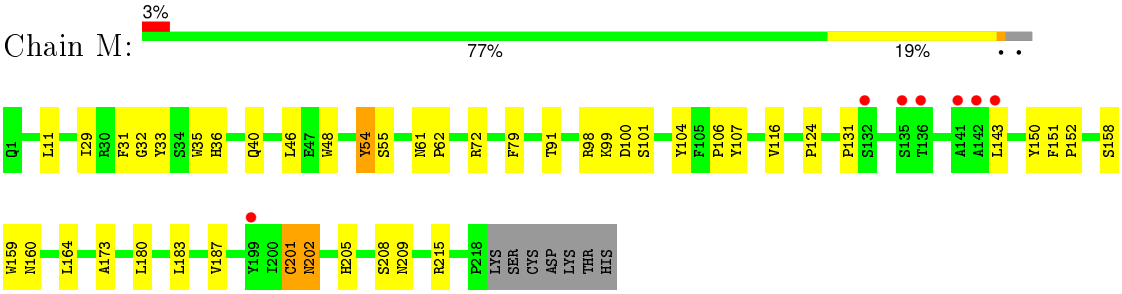
• Molecule 1: Fab C2E3 Heavy chain

Chain K:



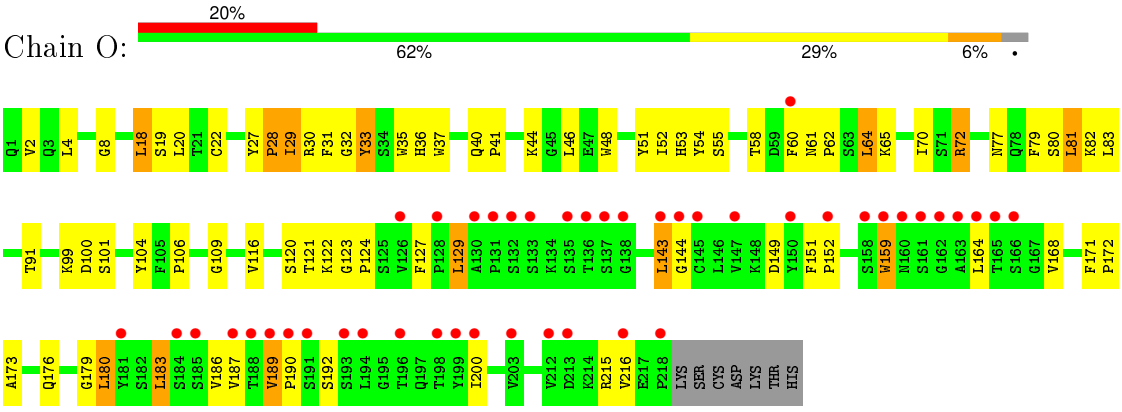
• Molecule 1: Fab C2E3 Heavy chain

Chain M:



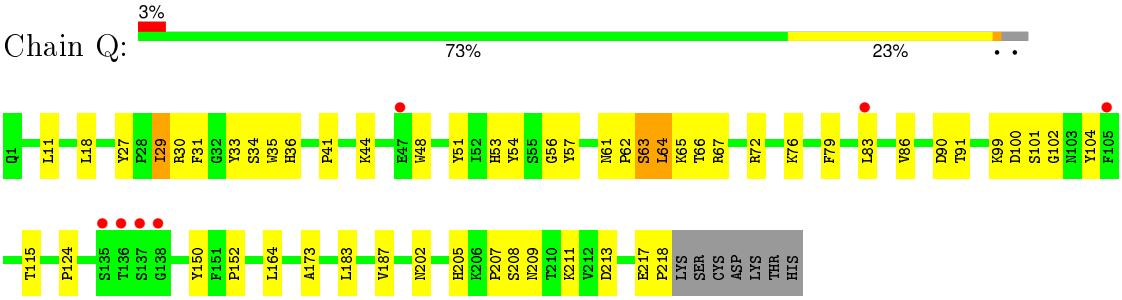
• Molecule 1: Fab C2E3 Heavy chain

Chain O:



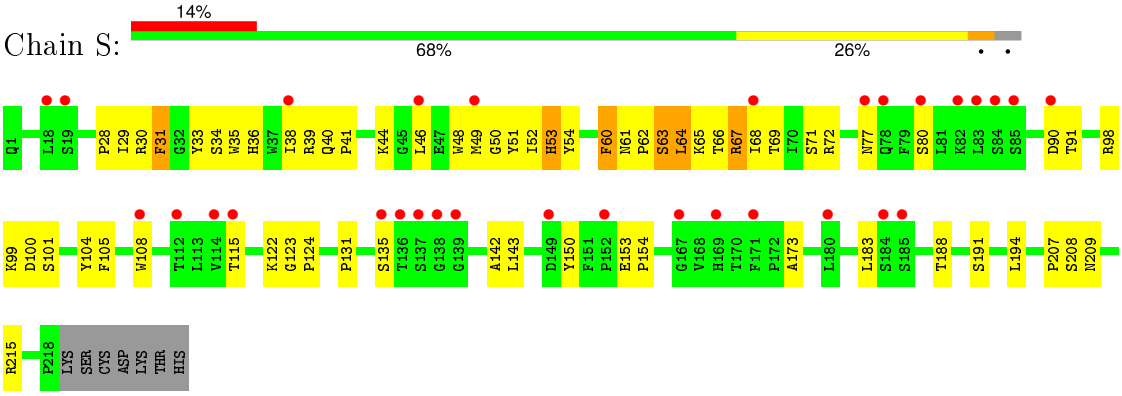
• Molecule 1: Fab C2E3 Heavy chain

Chain Q:



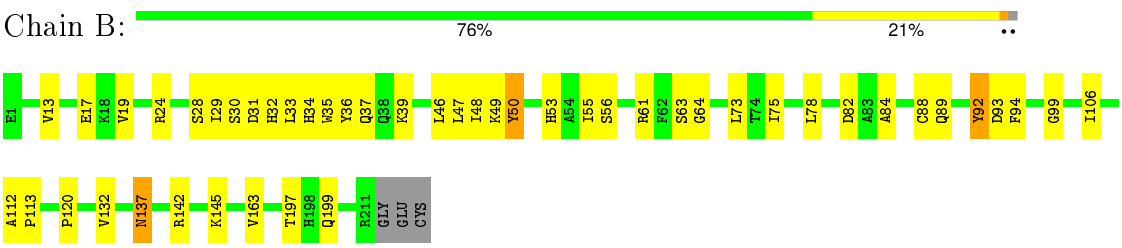
• Molecule 1: Fab C2E3 Heavy chain

Chain S:



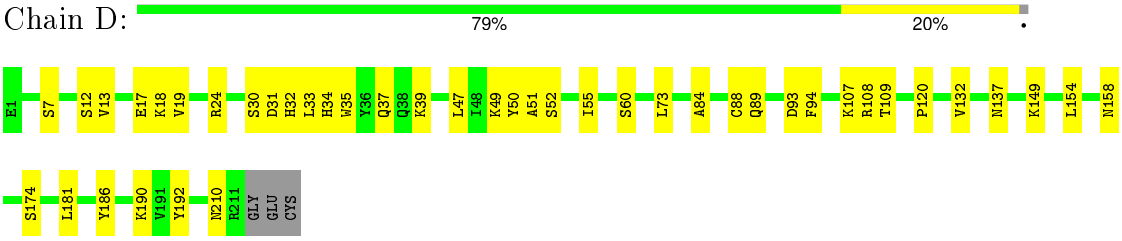
• Molecule 2: Fab C2E3 Light chain

Chain B:



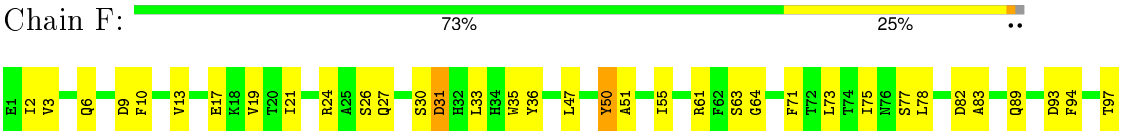
• Molecule 2: Fab C2E3 Light chain

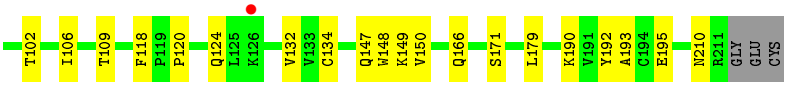
Chain D:



• Molecule 2: Fab C2E3 Light chain

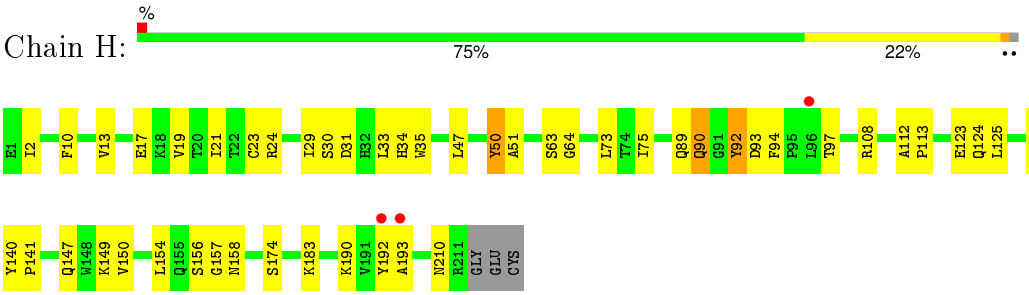
Chain F:





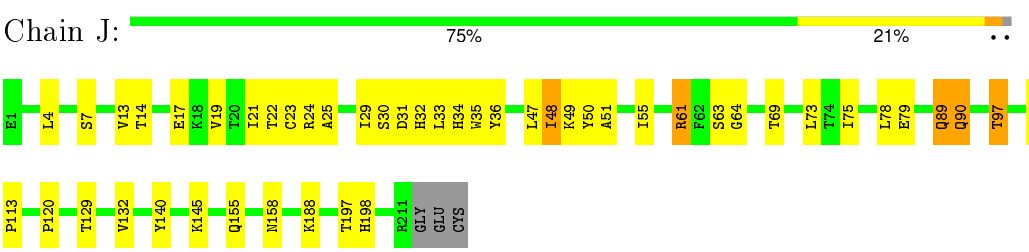
• Molecule 2: Fab C2E3 Light chain

Chain H:



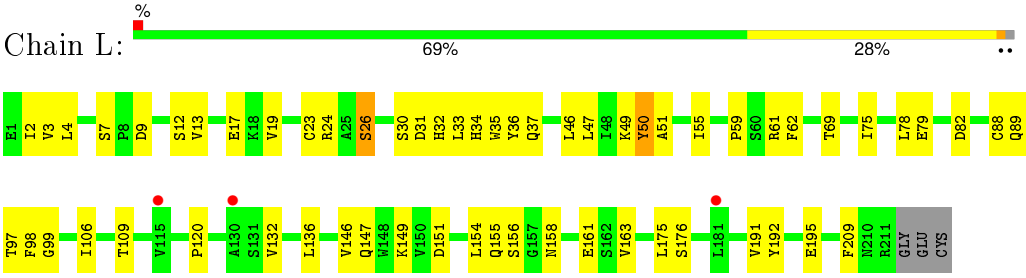
• Molecule 2: Fab C2E3 Light chain

Chain J:



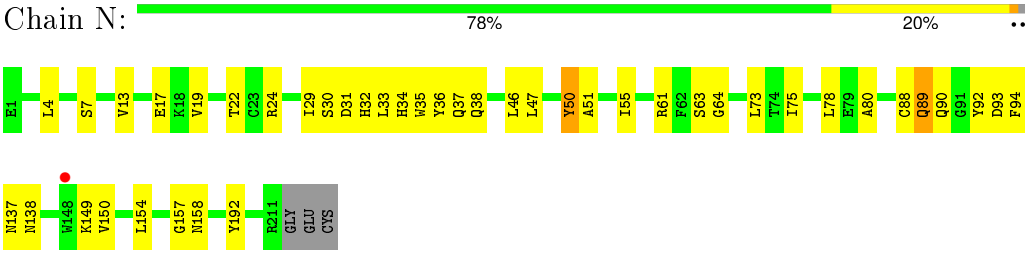
• Molecule 2: Fab C2E3 Light chain

Chain L:



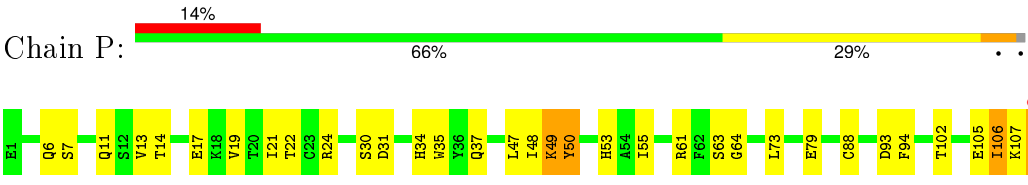
• Molecule 2: Fab C2E3 Light chain

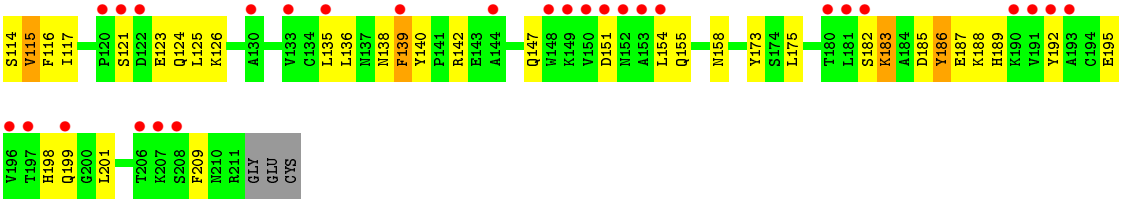
Chain N:



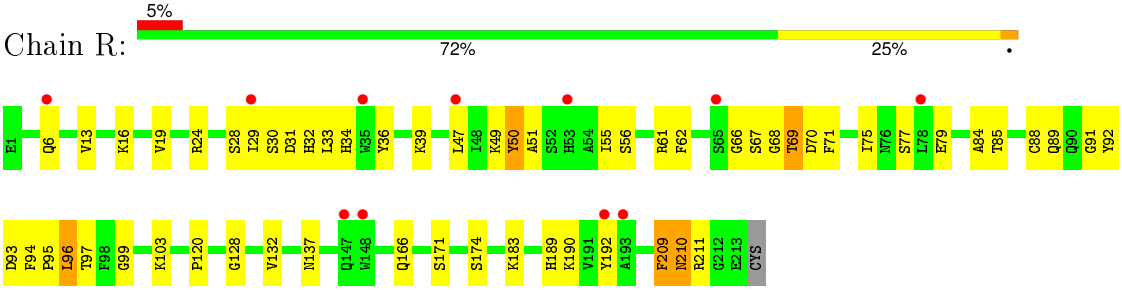
• Molecule 2: Fab C2E3 Light chain

Chain P:

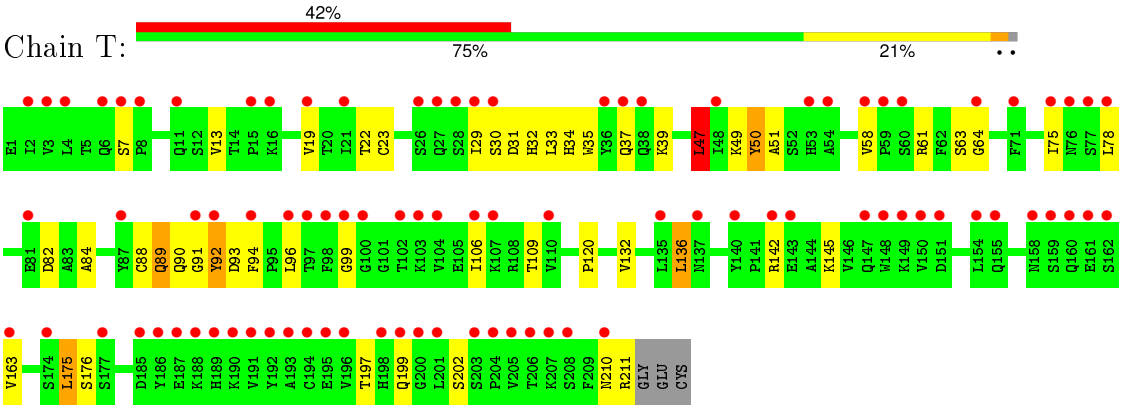




• Molecule 2: Fab C2E3 Light chain



• Molecule 2: Fab C2E3 Light chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	178.10Å 208.41Å 214.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.77 – 3.45 48.77 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.77-3.45) 100.0 (48.77-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.236 , 0.280 0.236 , 0.281	Depositor DCC
R_{free} test set	4999 reflections (4.75%)	DCC
Wilson B-factor (Å^2)	101.8	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 93.5	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 105335 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32933	wwPDB-VP
Average B, all atoms (Å^2)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.59 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5095e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.26	0/1705	0.51	0/2330
1	C	0.26	0/1705	0.51	1/2330 (0.0%)
1	E	0.27	0/1705	0.50	0/2330
1	G	0.25	0/1705	0.49	0/2330
1	I	0.27	0/1705	0.49	0/2330
1	K	0.26	0/1705	0.49	0/2330
1	M	0.26	0/1705	0.50	0/2330
1	O	0.34	0/1705	0.52	0/2330
1	Q	0.25	0/1705	0.48	0/2330
1	S	0.26	0/1705	0.50	0/2330
2	B	0.26	0/1672	0.45	0/2271
2	D	0.26	0/1672	0.47	0/2271
2	F	0.24	0/1672	0.46	1/2271 (0.0%)
2	H	0.25	0/1672	0.45	0/2271
2	J	0.25	0/1672	0.46	0/2271
2	L	0.26	0/1672	0.47	1/2271 (0.0%)
2	N	0.24	0/1672	0.45	0/2271
2	P	0.32	0/1672	0.53	0/2271
2	R	0.27	0/1685	0.49	1/2288 (0.0%)
2	T	0.23	0/1672	0.48	3/2271 (0.1%)
All	All	0.26	0/33783	0.48	7/46027 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	175	LEU	CA-CB-CG	6.26	129.71	115.30
2	T	47	LEU	CA-CB-CG	5.39	127.71	115.30
2	R	50	TYR	N-CA-C	5.36	125.46	111.00
2	T	50	TYR	N-CA-C	5.35	125.45	111.00
2	L	50	TYR	N-CA-C	5.25	125.17	111.00
2	F	50	TYR	N-CA-C	5.07	124.68	111.00
1	C	32	GLY	N-CA-C	5.01	125.63	113.10

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	1657	0	1625	44	0
1	C	1657	0	1625	33	0
1	E	1657	0	1625	50	0
1	G	1657	0	1625	37	0
1	I	1657	0	1625	29	0
1	K	1657	0	1625	42	0
1	M	1657	0	1625	40	0
1	O	1657	0	1629	60	0
1	Q	1657	0	1625	43	0
1	S	1657	0	1625	47	0
2	B	1635	0	1587	30	0
2	D	1635	0	1587	32	0
2	F	1635	0	1587	40	0
2	H	1635	0	1587	36	0
2	J	1635	0	1587	39	0
2	L	1635	0	1587	46	0
2	N	1635	0	1587	34	0
2	P	1635	0	1587	65	0
2	R	1648	0	1596	47	0
2	T	1635	0	1587	32	0
All	All	32933	0	32133	772	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 12.

All (772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:PRO:HB3	1:K:150:TYR:HB3	1.51	0.93
1:E:36:HIS:HD2	1:E:48:TRP:HE1	1.17	0.89
2:B:29:ILE:HA	2:B:92:TYR:HD2	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:49:LYS:HE3	2:J:50:TYR:CE2	2.09	0.88
2:H:29:ILE:HA	2:H:92:TYR:HD2	1.39	0.86
1:E:36:HIS:CE1	1:E:99:LYS:HB2	2.13	0.84
1:E:129:LEU:HD22	1:E:144:GLY:H	1.40	0.84
2:T:90:GLN:HE22	2:T:96:LEU:HA	1.44	0.83
1:E:27:TYR:HE2	1:E:32:GLY:HA3	1.45	0.82
1:C:124:PRO:HB3	1:C:150:TYR:HB3	1.60	0.82
1:K:36:HIS:CE1	1:K:99:LYS:HB2	2.15	0.82
1:I:36:HIS:NE2	1:I:99:LYS:HB2	1.96	0.81
1:O:91:THR:HG22	1:O:116:VAL:H	1.45	0.80
2:N:90:GLN:NE2	2:N:93:ASP:O	2.14	0.80
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.63	0.79
1:S:54:TYR:O	1:S:72:ARG:NH1	2.16	0.78
2:J:49:LYS:HE3	2:J:50:TYR:CZ	2.19	0.77
2:R:189:HIS:O	2:R:211:ARG:NH2	2.18	0.77
2:B:30:SER:OG	2:B:31:ASP:N	2.18	0.77
1:C:61:ASN:ND2	1:C:62:PRO:O	2.18	0.76
2:P:61:ARG:NH1	2:P:79:GLU:OE1	2.18	0.76
2:R:30:SER:N	2:R:68:GLY:O	2.19	0.76
2:P:14:THR:HA	2:P:107:LYS:HG3	1.66	0.75
2:L:136:LEU:HD12	2:L:175:LEU:HB3	1.69	0.75
1:I:164:LEU:HD21	1:I:187:VAL:HG21	1.69	0.75
2:L:163:VAL:HG22	2:L:175:LEU:HG	1.69	0.74
1:I:124:PRO:HB3	1:I:150:TYR:HB3	1.68	0.74
1:M:36:HIS:NE2	1:M:99:LYS:HB2	2.03	0.74
1:C:51:TYR:HE1	1:C:59:ASP:HB3	1.53	0.74
2:F:6:GLN:HE21	2:F:102:THR:HG23	1.53	0.74
1:M:91:THR:HG22	1:M:116:VAL:H	1.52	0.73
1:O:36:HIS:NE2	1:O:99:LYS:HB2	2.03	0.73
2:T:37:GLN:HB2	2:T:47:LEU:HD21	1.70	0.73
1:Q:36:HIS:NE2	1:Q:99:LYS:HB2	2.03	0.73
2:P:6:GLN:HE21	2:P:102:THR:HG23	1.52	0.73
1:G:33:TYR:O	1:G:35:TRP:NE1	2.22	0.73
1:Q:67:ARG:NH2	1:Q:90:ASP:OD2	2.21	0.72
2:P:30:SER:OG	2:P:31:ASP:N	2.21	0.72
1:A:36:HIS:NE2	1:A:99:LYS:HB2	2.04	0.72
1:K:164:LEU:HD21	1:K:187:VAL:HG21	1.71	0.71
1:S:41:PRO:HG2	1:S:44:LYS:HB2	1.73	0.71
1:M:208:SER:O	1:S:215:ARG:NH1	2.24	0.71
1:G:36:HIS:NE2	1:G:99:LYS:HB2	2.06	0.71
2:L:161:GLU:HB3	2:L:175:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ARG:NH1	1:C:90:ASP:OD2	2.22	0.71
1:G:29:ILE:HG22	1:G:35:TRP:CE2	2.25	0.70
1:A:41:PRO:HG2	1:A:44:LYS:HB2	1.73	0.70
2:L:30:SER:OG	2:L:31:ASP:N	2.24	0.70
2:H:30:SER:OG	2:H:31:ASP:N	2.25	0.70
1:K:36:HIS:HD2	1:K:48:TRP:HE1	1.39	0.70
2:P:151:ASP:OD2	2:P:189:HIS:ND1	2.25	0.70
1:O:33:TYR:H	1:O:33:TYR:HD1	1.39	0.70
2:L:36:TYR:HE2	2:L:89:GLN:HG2	1.56	0.70
1:E:36:HIS:CD2	1:E:48:TRP:HE1	2.05	0.70
2:H:29:ILE:HA	2:H:92:TYR:CD2	2.24	0.69
2:F:30:SER:OG	2:F:31:ASP:N	2.24	0.69
1:S:36:HIS:HE2	1:S:99:LYS:HB2	1.58	0.68
2:R:120:PRO:HD3	2:R:132:VAL:HG22	1.75	0.68
1:A:40:GLN:HB2	1:A:46:LEU:HD23	1.76	0.68
1:A:33:TYR:O	1:A:35:TRP:NE1	2.27	0.68
1:C:36:HIS:NE2	1:C:99:LYS:HB2	2.09	0.68
1:S:36:HIS:NE2	1:S:99:LYS:HB2	2.09	0.68
1:S:40:GLN:HB2	1:S:46:LEU:HD23	1.75	0.68
2:R:32:HIS:HB2	2:R:91:GLY:O	1.94	0.68
1:E:34:SER:HB2	1:E:36:HIS:HE1	1.58	0.67
2:F:21:ILE:HD12	2:F:73:LEU:HD23	1.75	0.67
2:P:7:SER:HG	2:P:22:THR:HG1	1.43	0.67
2:N:36:TYR:HE1	2:N:89:GLN:HG2	1.59	0.67
1:K:36:HIS:CD2	1:K:48:TRP:HE1	2.12	0.67
2:P:21:ILE:HD12	2:P:73:LEU:HD23	1.76	0.67
1:Q:61:ASN:O	1:Q:65:LYS:HG3	1.95	0.66
1:O:22:CYS:HB3	1:O:79:PHE:HB2	1.77	0.66
2:P:155:GLN:OE1	2:P:158:ASN:ND2	2.29	0.66
1:K:48:TRP:HZ2	1:K:51:TYR:HD2	1.43	0.66
1:E:40:GLN:HB2	1:E:46:LEU:HD13	1.78	0.66
1:O:53:HIS:HE1	1:O:54:TYR:CE2	2.13	0.66
1:G:103:ASN:O	2:H:89:GLN:NE2	2.29	0.66
2:R:28:SER:HA	2:R:69:THR:OG1	1.96	0.66
1:E:32:GLY:H	1:E:54:TYR:HD2	1.44	0.65
2:B:46:LEU:HG	2:B:55:ILE:HG13	1.77	0.65
1:O:120:SER:OG	1:O:121:THR:N	2.29	0.65
1:G:91:THR:HG23	1:G:115:THR:HA	1.78	0.65
1:G:98:ARG:NH1	1:G:100:ASP:OD2	2.30	0.65
1:M:54:TYR:HD1	1:M:55:SER:N	1.95	0.65
2:N:24:ARG:NH2	2:P:17:GLU:OE2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:8:GLY:HA3	1:O:20:LEU:HD23	1.78	0.64
1:O:149:ASP:HA	1:O:180:LEU:HB3	1.79	0.64
1:M:29:ILE:HG22	1:M:35:TRP:CE2	2.32	0.64
2:L:93:ASP:OD1	2:L:94:PHE:N	2.30	0.64
2:R:192:TYR:HB2	2:R:209:PHE:CE1	2.33	0.64
1:S:64:LEU:HD22	1:S:67:ARG:HH21	1.63	0.64
2:R:192:TYR:HB2	2:R:209:PHE:HE1	1.61	0.64
1:G:48:TRP:HZ2	1:G:51:TYR:HD2	1.44	0.64
1:G:40:GLN:HB2	1:G:46:LEU:HD23	1.80	0.64
1:S:124:PRO:HB3	1:S:150:TYR:HB3	1.78	0.64
1:E:144:GLY:HA3	1:E:186:VAL:HA	1.79	0.64
1:I:91:THR:HG23	1:I:115:THR:HA	1.79	0.64
2:B:17:GLU:OE2	2:J:24:ARG:NH2	2.30	0.64
2:H:24:ARG:NH2	2:L:17:GLU:OE2	2.31	0.64
1:G:204:ASN:HD21	1:G:206:LYS:HE2	1.63	0.63
1:C:104:TYR:CE2	2:D:49:LYS:HD3	2.33	0.63
1:M:160:ASN:HD22	1:M:164:LEU:HD13	1.63	0.63
1:M:159:TRP:HZ3	1:M:187:VAL:HB	1.64	0.63
2:R:137:ASN:O	2:R:174:SER:OG	2.14	0.63
1:O:36:HIS:HE2	1:O:99:LYS:HB2	1.62	0.63
2:J:21:ILE:HD12	2:J:73:LEU:HD23	1.81	0.63
1:Q:30:ARG:HA	1:Q:54:TYR:HB2	1.80	0.63
1:M:33:TYR:O	1:M:35:TRP:NE1	2.31	0.62
1:G:61:ASN:OD1	1:G:63:SER:OG	2.14	0.62
1:O:33:TYR:N	1:O:33:TYR:CD1	2.67	0.62
2:F:61:ARG:NH2	2:F:82:ASP:OD1	2.27	0.62
1:K:36:HIS:HE1	1:K:99:LYS:HB2	1.61	0.62
1:I:51:TYR:HE1	1:I:59:ASP:HB3	1.64	0.62
1:S:29:ILE:HG13	1:S:77:ASN:OD1	2.00	0.62
1:A:98:ARG:HH21	1:A:106:PRO:HG3	1.65	0.62
2:H:17:GLU:OE2	2:L:24:ARG:NH2	2.31	0.62
2:P:115:VAL:HG12	2:P:136:LEU:HA	1.82	0.62
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.81	0.62
1:M:40:GLN:HB3	1:M:46:LEU:HD23	1.81	0.62
1:A:91:THR:HG23	1:A:115:THR:HA	1.82	0.62
1:O:27:TYR:OH	1:O:32:GLY:HA3	1.99	0.62
2:F:50:TYR:N	2:F:51:ALA:HA	2.15	0.62
1:S:29:ILE:O	1:S:54:TYR:HB3	2.01	0.61
1:S:67:ARG:NH1	1:S:90:ASP:OD2	2.29	0.61
1:E:29:ILE:HG22	1:E:35:TRP:CE2	2.35	0.61
2:B:36:TYR:HE1	2:B:89:GLN:HG2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:SER:OG	1:C:121:THR:N	2.34	0.61
2:D:17:GLU:OE2	2:F:24:ARG:NH2	2.32	0.61
1:S:33:TYR:O	1:S:35:TRP:NE1	2.33	0.61
2:R:50:TYR:N	2:R:51:ALA:HA	2.15	0.61
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.33	0.61
2:F:148:TRP:CD2	2:F:179:LEU:HD23	2.36	0.61
1:O:41:PRO:HB2	1:O:44:LYS:HE2	1.83	0.61
2:H:50:TYR:N	2:H:51:ALA:HA	2.16	0.61
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.82	0.61
1:O:159:TRP:HZ3	1:O:164:LEU:HD13	1.66	0.61
2:B:29:ILE:HA	2:B:92:TYR:CD2	2.26	0.60
1:O:48:TRP:HZ2	1:O:51:TYR:HD2	1.48	0.60
2:L:50:TYR:N	2:L:51:ALA:HA	2.15	0.60
2:L:147:GLN:HB3	2:L:195:GLU:HB3	1.83	0.60
1:S:29:ILE:HD12	1:S:30:ARG:H	1.65	0.60
2:F:3:VAL:N	2:F:26:SER:OG	2.27	0.60
1:G:54:TYR:HD1	1:G:55:SER:N	1.98	0.60
2:P:106:ILE:H	2:P:106:ILE:HD12	1.66	0.60
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.84	0.60
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.84	0.60
2:P:107:LYS:HD3	2:P:109:THR:HB	1.84	0.60
2:P:125:LEU:HG	2:P:183:LYS:HD3	1.84	0.59
1:E:61:ASN:HD22	1:E:64:LEU:HD23	1.66	0.59
2:R:30:SER:OG	2:R:31:ASP:N	2.35	0.59
1:M:159:TRP:CZ3	1:M:187:VAL:HB	2.37	0.59
2:P:105:GLU:HG3	2:P:106:ILE:H	1.66	0.59
1:M:124:PRO:HB3	1:M:150:TYR:HB3	1.85	0.59
1:M:215:ARG:NH2	1:S:209:ASN:H	1.98	0.59
2:B:24:ARG:NH2	2:J:17:GLU:OE2	2.35	0.59
2:P:34:HIS:HE1	2:P:50:TYR:HD2	1.49	0.59
2:H:137:ASN:O	2:H:174:SER:OG	2.11	0.59
1:C:104:TYR:CZ	2:D:49:LYS:HD3	2.37	0.59
2:L:3:VAL:N	2:L:26:SER:OG	2.31	0.59
2:F:190:LYS:HE3	2:F:210:ASN:HB3	1.85	0.59
2:T:50:TYR:N	2:T:51:ALA:HA	2.18	0.59
1:O:60:PHE:HB2	1:O:65:LYS:HG3	1.83	0.59
1:I:36:HIS:HE2	1:I:99:LYS:HB2	1.67	0.58
2:T:120:PRO:HD3	2:T:132:VAL:HG22	1.86	0.58
2:P:105:GLU:HG3	2:P:106:ILE:HD12	1.84	0.58
1:I:149:ASP:HA	1:I:180:LEU:HB3	1.85	0.58
1:S:91:THR:HG23	1:S:115:THR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:TYR:O	1:O:72:ARG:NH2	2.34	0.58
1:C:62:PRO:O	1:C:63:SER:OG	2.21	0.58
2:P:11:GLN:O	2:P:105:GLU:N	2.31	0.58
1:O:173:ALA:HA	1:O:183:LEU:HD13	1.85	0.58
1:E:11:LEU:HB3	1:E:152:PRO:HG3	1.86	0.58
2:J:19:VAL:HB	2:J:75:ILE:HB	1.84	0.58
2:R:36:TYR:OH	2:R:89:GLN:NE2	2.36	0.58
1:K:11:LEU:HB2	1:K:152:PRO:HG3	1.86	0.58
1:Q:61:ASN:OD1	1:Q:63:SER:OG	2.21	0.57
1:K:91:THR:HG23	1:K:115:THR:HA	1.85	0.57
1:O:40:GLN:HB2	1:O:46:LEU:HD23	1.86	0.57
1:S:67:ARG:NH2	1:S:90:ASP:OD1	2.34	0.57
2:D:50:TYR:N	2:D:51:ALA:HA	2.20	0.57
2:N:30:SER:OG	2:N:31:ASP:N	2.35	0.57
1:S:100:ASP:OD1	1:S:101:SER:N	2.35	0.57
2:N:137:ASN:OD1	2:N:138:ASN:ND2	2.29	0.57
1:Q:29:ILE:HD12	1:Q:30:ARG:H	1.69	0.57
1:S:123:GLY:H	1:S:124:PRO:HD3	1.70	0.57
1:G:164:LEU:HD21	1:G:187:VAL:HG21	1.87	0.57
1:C:202:ASN:ND2	1:C:213:ASP:OD2	2.37	0.57
2:J:78:LEU:HD11	2:J:106:ILE:HG12	1.87	0.57
2:T:34:HIS:HD2	2:T:89:GLN:HE21	1.52	0.57
1:Q:91:THR:HG23	1:Q:115:THR:HA	1.87	0.57
2:N:50:TYR:N	2:N:51:ALA:HA	2.20	0.57
2:P:198:HIS:H	2:P:201:LEU:HD11	1.70	0.57
2:J:50:TYR:N	2:J:51:ALA:HA	2.20	0.57
1:O:81:LEU:HD12	1:O:82:LYS:N	2.20	0.57
2:L:49:LYS:HG2	2:L:50:TYR:HD2	1.69	0.57
1:S:30:ARG:HA	1:S:54:TYR:HB2	1.87	0.56
1:E:48:TRP:HZ2	1:E:51:TYR:HD2	1.54	0.56
1:O:53:HIS:CE1	1:O:54:TYR:CE2	2.94	0.56
1:I:40:GLN:HB2	1:I:46:LEU:HD23	1.87	0.56
1:Q:100:ASP:OD1	1:Q:101:SER:N	2.34	0.56
1:M:33:TYR:CD1	1:M:98:ARG:HD2	2.41	0.56
1:Q:164:LEU:HD21	1:Q:187:VAL:HG21	1.86	0.56
2:R:190:LYS:HE2	2:R:210:ASN:HB3	1.87	0.56
2:F:13:VAL:HB	2:F:78:LEU:HD22	1.86	0.56
2:T:136:LEU:HD11	2:T:175:LEU:HB3	1.86	0.56
2:F:19:VAL:HB	2:F:75:ILE:HB	1.88	0.56
2:J:33:LEU:HB3	2:J:51:ALA:HB2	1.86	0.56
1:A:36:HIS:HE2	1:A:99:LYS:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:54:TYR:O	1:Q:72:ARG:NH1	2.38	0.56
1:C:100:ASP:OD1	1:C:101:SER:N	2.38	0.56
2:B:93:ASP:OD1	2:B:94:PHE:N	2.38	0.56
2:B:88:CYS:O	2:B:99:GLY:N	2.38	0.56
1:Q:36:HIS:HE2	1:Q:99:LYS:HB2	1.69	0.56
2:B:36:TYR:CE1	2:B:89:GLN:HG2	2.41	0.55
1:A:61:ASN:ND2	1:A:63:SER:OG	2.39	0.55
1:A:100:ASP:OD1	1:A:101:SER:N	2.37	0.55
1:E:98:ARG:HG2	1:E:100:ASP:H	1.71	0.55
1:C:148:LYS:NZ	1:C:176:GLN:OE1	2.34	0.55
2:T:30:SER:OG	2:T:31:ASP:N	2.39	0.55
2:P:6:GLN:NE2	2:P:102:THR:HG23	2.21	0.55
2:N:19:VAL:HB	2:N:75:ILE:HB	1.89	0.55
2:R:16:LYS:HA	2:R:77:SER:HB2	1.89	0.55
2:J:4:LEU:HD21	2:J:90:GLN:HG3	1.87	0.55
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.40	0.55
1:E:36:HIS:HE1	1:E:99:LYS:HB2	1.70	0.55
1:S:29:ILE:HD12	1:S:30:ARG:N	2.21	0.55
2:T:47:LEU:HA	2:T:58:VAL:HG11	1.88	0.55
1:K:98:ARG:HH21	1:K:107:TYR:HE2	1.54	0.55
1:K:53:HIS:HD2	1:K:57:TYR:CE2	2.24	0.55
2:R:93:ASP:OD1	2:R:94:PHE:N	2.40	0.55
2:B:19:VAL:HB	2:B:75:ILE:HB	1.88	0.55
1:E:131:PRO:HG2	1:E:218:PRO:HG3	1.89	0.55
1:A:54:TYR:O	1:A:72:ARG:NH1	2.33	0.55
1:A:123:GLY:H	1:A:124:PRO:HD3	1.72	0.54
2:P:114:SER:H	2:P:138:ASN:HB2	1.70	0.54
1:Q:202:ASN:ND2	1:Q:213:ASP:OD2	2.40	0.54
2:D:190:LYS:HE3	2:D:210:ASN:HB3	1.87	0.54
1:S:50:GLY:HA3	1:S:60:PHE:HA	1.88	0.54
1:E:18:LEU:HB3	1:E:83:LEU:HB3	1.89	0.54
1:E:33:TYR:O	1:E:35:TRP:NE1	2.41	0.54
1:S:153:GLU:HG2	1:S:154:PRO:HA	1.89	0.54
1:K:34:SER:HB2	1:K:36:HIS:HE1	1.73	0.54
1:O:28:PRO:HG2	1:O:31:PHE:HD2	1.71	0.54
1:S:48:TRP:CE3	1:S:61:ASN:HB2	2.42	0.54
1:M:152:PRO:O	1:M:205:HIS:NE2	2.41	0.54
2:L:89:GLN:HB3	2:L:98:PHE:CD1	2.43	0.54
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.89	0.54
1:O:32:GLY:O	1:O:54:TYR:CD2	2.61	0.54
2:N:46:LEU:HG	2:N:55:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:LEU:HD21	2:N:90:GLN:HB3	1.90	0.53
2:B:55:ILE:O	2:B:56:SER:HB3	2.08	0.53
1:Q:33:TYR:O	1:Q:35:TRP:NE1	2.41	0.53
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.88	0.53
2:T:136:LEU:HD11	2:T:175:LEU:HD22	1.90	0.53
2:H:19:VAL:HB	2:H:75:ILE:HB	1.90	0.53
1:E:72:ARG:HA	1:E:79:PHE:HA	1.90	0.53
1:A:180:LEU:HD21	1:G:30:ARG:HD2	1.89	0.53
2:P:192:TYR:HB2	2:P:209:PHE:HE1	1.72	0.53
2:P:139:PHE:HB3	2:P:173:TYR:HB2	1.88	0.53
2:D:33:LEU:HB3	2:D:51:ALA:HB2	1.90	0.53
1:O:4:LEU:HD22	1:O:109:GLY:HA3	1.89	0.53
1:A:142:ALA:HB2	1:A:188:THR:HG22	1.91	0.53
2:P:14:THR:HG22	2:P:107:LYS:HE3	1.90	0.53
1:I:33:TYR:HB2	1:I:98:ARG:HD2	1.90	0.53
2:T:136:LEU:CD1	2:T:175:LEU:HB3	2.39	0.53
2:F:6:GLN:NE2	2:F:102:THR:HG23	2.21	0.53
1:M:54:TYR:O	1:M:72:ARG:NH1	2.41	0.53
1:M:61:ASN:ND2	1:M:62:PRO:O	2.41	0.53
2:H:93:ASP:OD1	2:H:94:PHE:N	2.41	0.52
1:C:41:PRO:HB2	1:C:44:LYS:HB2	1.90	0.52
2:P:50:TYR:N	2:P:50:TYR:CD1	2.77	0.52
1:M:215:ARG:HH22	1:S:209:ASN:H	1.58	0.52
1:I:96:CYS:O	1:I:109:GLY:N	2.43	0.52
1:A:98:ARG:HH21	1:A:106:PRO:CG	2.22	0.52
2:P:115:VAL:CG1	2:P:136:LEU:HG	2.39	0.52
2:P:115:VAL:HG12	2:P:136:LEU:HG	1.92	0.52
2:P:108:ARG:HE	2:P:108:ARG:HA	1.75	0.52
1:K:191:SER:HA	1:K:194:LEU:HD13	1.90	0.52
2:L:32:HIS:ND1	2:L:50:TYR:HE1	2.08	0.52
2:D:108:ARG:NH1	2:D:109:THR:O	2.43	0.52
1:E:18:LEU:N	1:E:83:LEU:O	2.35	0.51
1:G:72:ARG:HA	1:G:79:PHE:HA	1.91	0.51
1:M:159:TRP:NE1	1:M:201:CYS:HB2	2.25	0.51
1:M:215:ARG:HH12	1:S:208:SER:HA	1.75	0.51
2:L:175:LEU:HD23	2:L:176:SER:N	2.25	0.51
2:F:149:LYS:HB2	2:F:193:ALA:HB3	1.91	0.51
2:N:78:LEU:HD11	2:N:106:ILE:HG12	1.92	0.51
2:F:83:ALA:HB2	2:F:106:ILE:HD13	1.91	0.51
1:G:11:LEU:HB2	1:G:152:PRO:HG3	1.93	0.51
1:M:202:ASN:N	1:M:202:ASN:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:SER:OG	2:B:64:GLY:N	2.43	0.51
1:E:54:TYR:O	1:E:72:ARG:NH1	2.42	0.51
1:M:11:LEU:HB3	1:M:152:PRO:HG3	1.93	0.51
2:T:19:VAL:HB	2:T:75:ILE:HB	1.92	0.51
1:Q:205:HIS:CD2	1:Q:207:PRO:HD2	2.46	0.51
2:T:61:ARG:NH2	2:T:82:ASP:OD1	2.44	0.51
2:R:47:LEU:HD21	2:R:62:PHE:HD2	1.76	0.51
1:O:143:LEU:HB2	1:O:216:VAL:HG11	1.92	0.51
1:O:37:TRP:CE2	1:O:81:LEU:HB3	2.46	0.51
1:S:38:ILE:HD12	1:S:108:TRP:CH2	2.46	0.51
1:Q:62:PRO:HD3	2:R:95:PRO:HG2	1.92	0.51
1:E:96:CYS:O	1:E:109:GLY:N	2.44	0.51
2:P:116:PHE:O	2:P:135:LEU:N	2.36	0.50
1:C:18:LEU:N	1:C:83:LEU:O	2.38	0.50
2:B:78:LEU:HD11	2:B:106:ILE:HG12	1.93	0.50
1:S:65:LYS:O	1:S:68:ILE:HG22	2.11	0.50
2:L:155:GLN:OE1	2:L:158:ASN:ND2	2.35	0.50
2:F:93:ASP:OD1	2:F:94:PHE:N	2.44	0.50
2:D:93:ASP:OD1	2:D:94:PHE:N	2.44	0.50
1:A:143:LEU:H	1:A:143:LEU:HD12	1.76	0.50
1:M:173:ALA:HB2	1:M:183:LEU:HD23	1.92	0.50
1:E:100:ASP:OD1	1:E:101:SER:N	2.43	0.50
1:K:104:TYR:HD1	2:L:46:LEU:HD11	1.76	0.50
1:A:32:GLY:O	1:A:54:TYR:HD2	1.94	0.50
1:Q:48:TRP:HZ2	1:Q:51:TYR:HD2	1.58	0.50
2:D:137:ASN:O	2:D:174:SER:OG	2.17	0.50
1:G:52:ILE:HG13	1:G:58:THR:HG22	1.92	0.50
2:T:90:GLN:NE2	2:T:96:LEU:HA	2.21	0.50
2:T:33:LEU:HB3	2:T:51:ALA:HB2	1.93	0.50
1:M:173:ALA:HA	1:M:183:LEU:HB3	1.94	0.50
2:J:63:SER:OG	2:J:64:GLY:N	2.45	0.50
1:K:33:TYR:N	1:K:33:TYR:CD1	2.80	0.50
2:P:93:ASP:OD1	2:P:94:PHE:N	2.44	0.50
2:P:34:HIS:HE1	2:P:50:TYR:CD2	2.28	0.50
2:R:61:ARG:CZ	2:R:79:GLU:HG3	2.42	0.50
1:Q:11:LEU:HB3	1:Q:152:PRO:HG3	1.94	0.50
1:S:173:ALA:HB2	1:S:183:LEU:HD23	1.94	0.50
2:H:63:SER:OG	2:H:64:GLY:N	2.45	0.50
1:G:148:LYS:NZ	1:G:176:GLN:OE1	2.38	0.50
2:H:156:SER:HB2	2:L:156:SER:HB2	1.92	0.50
1:O:33:TYR:HD2	1:O:100:ASP:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:104:TYR:HB3	2:N:34:HIS:CE1	2.47	0.49
1:O:2:VAL:HG22	1:O:27:TYR:HB2	1.94	0.49
2:R:66:GLY:HA3	2:R:71:PHE:HD1	1.75	0.49
1:M:40:GLN:NE2	2:N:38:GLN:OE1	2.39	0.49
1:C:72:ARG:HA	1:C:79:PHE:HA	1.94	0.49
1:C:173:ALA:HB2	1:C:183:LEU:HD23	1.93	0.49
1:C:33:TYR:O	1:C:35:TRP:NE1	2.45	0.49
2:P:21:ILE:HB	2:P:73:LEU:HB3	1.93	0.49
1:S:28:PRO:HA	1:S:77:ASN:HD21	1.75	0.49
1:A:122:LYS:HG2	1:A:123:GLY:HA3	1.93	0.49
1:E:91:THR:HG23	1:E:115:THR:HA	1.95	0.49
1:C:124:PRO:CB	1:C:150:TYR:HB3	2.36	0.49
1:O:164:LEU:HD11	1:O:189:VAL:HG21	1.95	0.49
2:F:78:LEU:HD21	2:F:106:ILE:HG13	1.94	0.49
1:Q:29:ILE:HG22	1:Q:35:TRP:CE2	2.47	0.49
1:O:127:PHE:CZ	2:P:124:GLN:HB3	2.48	0.49
2:T:145:LYS:HB3	2:T:197:THR:HB	1.95	0.49
2:R:19:VAL:HB	2:R:75:ILE:HB	1.94	0.49
1:K:48:TRP:HZ2	1:K:51:TYR:CD2	2.29	0.49
1:S:29:ILE:HG22	1:S:35:TRP:CE2	2.46	0.49
1:A:104:TYR:HB3	2:B:34:HIS:CE1	2.47	0.49
1:K:168:VAL:HG12	1:K:187:VAL:HB	1.94	0.49
1:C:30:ARG:HD2	1:M:180:LEU:HD21	1.93	0.49
2:L:136:LEU:HD11	2:L:146:VAL:CG2	2.43	0.49
1:Q:102:GLY:HA3	2:R:50:TYR:OH	2.13	0.49
2:T:93:ASP:OD1	2:T:94:PHE:N	2.45	0.49
2:L:151:ASP:HA	2:L:191:VAL:HG23	1.94	0.49
2:F:132:VAL:HB	2:F:179:LEU:HG	1.94	0.49
1:G:100:ASP:OD1	1:G:101:SER:N	2.40	0.49
1:E:129:LEU:CD2	1:E:144:GLY:H	2.18	0.48
2:R:128:GLY:HA2	2:R:183:LYS:HE2	1.94	0.48
1:I:11:LEU:HB3	1:I:152:PRO:HG3	1.95	0.48
2:R:47:LEU:HD21	2:R:62:PHE:CD2	2.47	0.48
1:Q:41:PRO:HB2	1:Q:44:LYS:HB2	1.94	0.48
2:F:61:ARG:HD2	2:F:77:SER:O	2.12	0.48
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.48	0.48
1:K:31:PHE:CD1	1:K:31:PHE:N	2.81	0.48
1:Q:34:SER:HB2	1:Q:53:HIS:HA	1.94	0.48
2:D:24:ARG:NH2	2:F:17:GLU:OE2	2.41	0.48
2:N:47:LEU:O	2:N:55:ILE:HG12	2.13	0.48
2:H:10:PHE:HB3	2:L:12:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:TYR:CG	1:G:98:ARG:HD3	2.48	0.48
2:R:66:GLY:HA3	2:R:71:PHE:CD1	2.48	0.48
1:A:153:GLU:HG2	1:A:154:PRO:HA	1.94	0.48
2:P:49:LYS:HD3	2:P:50:TYR:CE1	2.49	0.48
1:O:129:LEU:HD22	1:O:144:GLY:H	1.79	0.48
1:Q:208:SER:OG	1:Q:209:ASN:N	2.46	0.48
1:A:39:ARG:HD3	1:A:49:MET:HE3	1.96	0.48
2:T:63:SER:OG	2:T:64:GLY:N	2.46	0.48
2:P:199:GLN:OE1	2:P:199:GLN:N	2.46	0.48
1:G:29:ILE:HG13	1:G:29:ILE:H	1.45	0.48
2:H:2:ILE:HD12	2:H:90:GLN:OE1	2.14	0.48
1:M:159:TRP:CD1	1:M:201:CYS:HA	2.49	0.48
1:E:127:PHE:CE1	2:F:124:GLN:HG2	2.48	0.48
2:N:7:SER:HB2	2:P:13:VAL:HG23	1.96	0.48
2:P:13:VAL:HG21	2:P:19:VAL:HG22	1.95	0.48
1:G:96:CYS:O	1:G:109:GLY:N	2.47	0.48
1:I:104:TYR:CG	2:J:49:LYS:HD2	2.49	0.47
2:J:34:HIS:CE1	2:J:49:LYS:HZ3	2.32	0.47
1:S:33:TYR:HB2	1:S:98:ARG:HG3	1.96	0.47
2:R:36:TYR:HE1	2:R:89:GLN:HG2	1.78	0.47
1:E:41:PRO:HB2	1:E:44:LYS:HB2	1.96	0.47
1:O:18:LEU:HD22	1:O:19:SER:N	2.29	0.47
2:B:48:ILE:HG22	2:B:49:LYS:O	2.13	0.47
2:J:90:GLN:OE1	2:J:97:THR:N	2.41	0.47
2:N:63:SER:OG	2:N:64:GLY:N	2.46	0.47
2:H:149:LYS:HB2	2:H:193:ALA:HB3	1.97	0.47
1:E:27:TYR:CE2	1:E:32:GLY:HA3	2.37	0.47
2:P:136:LEU:HD22	2:P:139:PHE:CE1	2.50	0.47
2:P:49:LYS:O	2:P:53:HIS:HB2	2.13	0.47
2:N:35:TRP:CE2	2:N:73:LEU:HB2	2.50	0.47
2:D:186:TYR:O	2:D:192:TYR:OH	2.31	0.47
2:R:96:LEU:HD23	2:R:97:THR:H	1.78	0.47
1:K:124:PRO:CB	1:K:150:TYR:HB3	2.33	0.47
1:E:129:LEU:HG	1:E:130:ALA:N	2.27	0.47
1:O:33:TYR:CD2	1:O:100:ASP:HA	2.49	0.47
1:S:36:HIS:CG	1:S:105:PHE:HE2	2.31	0.47
2:H:21:ILE:HD12	2:H:73:LEU:HD23	1.97	0.47
2:P:63:SER:OG	2:P:64:GLY:N	2.47	0.47
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.47
1:O:100:ASP:OD1	1:O:101:SER:N	2.46	0.47
1:I:72:ARG:HA	1:I:79:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:36:TYR:HE2	2:J:89:GLN:HG2	1.79	0.47
1:I:2:VAL:HG22	1:I:27:TYR:HB2	1.95	0.47
2:T:7:SER:HG	2:T:22:THR:HG1	1.62	0.47
1:O:18:LEU:O	1:O:83:LEU:N	2.40	0.47
2:F:33:LEU:HG	2:F:71:PHE:CD2	2.50	0.47
1:S:52:ILE:HG12	1:S:53:HIS:O	2.14	0.47
2:J:47:LEU:HB3	2:J:48:ILE:HG12	1.96	0.47
2:N:29:ILE:HA	2:N:92:TYR:CD2	2.50	0.47
1:Q:18:LEU:HB2	1:Q:86:VAL:HG11	1.96	0.47
2:R:13:VAL:HG21	2:R:19:VAL:HG22	1.95	0.47
2:B:145:LYS:HB3	2:B:197:THR:HB	1.96	0.47
1:A:173:ALA:HB2	1:A:183:LEU:HD23	1.96	0.47
2:P:186:TYR:CE2	2:P:187:GLU:HG2	2.49	0.47
2:F:2:ILE:O	2:F:97:THR:HG21	2.15	0.47
1:A:135:SER:HA	1:A:191:SER:OG	2.14	0.47
1:K:131:PRO:HG3	1:K:143:LEU:HB3	1.95	0.47
1:G:104:TYR:HB3	2:H:34:HIS:CE1	2.49	0.47
2:T:199:GLN:OE1	2:T:199:GLN:N	2.45	0.47
2:L:46:LEU:HD22	2:L:55:ILE:HG12	1.96	0.47
2:N:80:ALA:HA	2:N:106:ILE:HD13	1.97	0.47
1:E:71:SER:O	1:E:80:SER:N	2.42	0.47
1:E:142:ALA:HB2	1:E:188:THR:HG22	1.96	0.47
2:J:13:VAL:HG21	2:J:19:VAL:HG22	1.97	0.47
1:K:153:GLU:HG2	1:K:154:PRO:HA	1.96	0.47
2:B:33:LEU:O	2:B:50:TYR:HA	2.15	0.47
1:O:189:VAL:HG22	1:O:190:PRO:HD2	1.97	0.46
2:J:23:CYS:HB2	2:J:35:TRP:CH2	2.51	0.46
2:T:13:VAL:HG21	2:T:19:VAL:HG22	1.97	0.46
1:C:35:TRP:CZ3	1:C:98:ARG:HD2	2.50	0.46
2:J:47:LEU:O	2:J:55:ILE:HG12	2.14	0.46
1:O:176:GLN:H	1:O:176:GLN:CD	2.18	0.46
1:O:70:ILE:HG23	1:O:80:SER:O	2.15	0.46
1:A:31:PHE:CD1	1:A:31:PHE:N	2.82	0.46
2:J:113:PRO:HD3	2:J:198:HIS:ND1	2.29	0.46
1:E:48:TRP:HZ2	1:E:51:TYR:CD2	2.33	0.46
1:M:32:GLY:O	1:M:54:TYR:CD2	2.67	0.46
1:S:62:PRO:O	1:S:65:LYS:HB2	2.14	0.46
2:P:182:SER:O	2:P:186:TYR:HB3	2.16	0.46
2:J:61:ARG:NH2	2:J:79:GLU:HG3	2.31	0.46
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.49	0.46
2:H:128:GLY:HA2	2:H:183:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:13:VAL:HG21	2:L:19:VAL:HG22	1.96	0.46
2:N:13:VAL:HG21	2:N:19:VAL:HG22	1.98	0.46
1:O:18:LEU:N	1:O:83:LEU:O	2.36	0.46
2:H:190:LYS:HE3	2:H:210:ASN:HB3	1.97	0.46
1:G:214:LYS:NZ	2:H:123:GLU:OE1	2.39	0.46
2:P:136:LEU:N	2:P:175:LEU:O	2.35	0.46
1:M:131:PRO:HG3	1:M:143:LEU:HB3	1.97	0.46
2:D:13:VAL:HG21	2:D:19:VAL:HG22	1.97	0.46
1:Q:72:ARG:HA	1:Q:79:PHE:HA	1.97	0.46
1:C:88:ALA:O	1:C:91:THR:HG22	2.16	0.46
1:E:129:LEU:HD23	1:E:143:LEU:HB2	1.97	0.46
1:S:142:ALA:HB2	1:S:188:THR:HG22	1.98	0.46
2:P:49:LYS:HG3	2:P:55:ILE:HD11	1.98	0.46
2:F:47:LEU:O	2:F:55:ILE:HG12	2.15	0.46
1:G:18:LEU:N	1:G:83:LEU:O	2.37	0.46
2:L:149:LYS:HG2	2:L:154:LEU:HD23	1.97	0.46
2:J:34:HIS:CE1	2:J:49:LYS:NZ	2.83	0.46
1:C:48:TRP:CE3	1:C:61:ASN:HB2	2.51	0.46
1:C:102:GLY:HA3	2:D:50:TYR:OH	2.15	0.46
1:S:61:ASN:OD1	1:S:63:SER:N	2.48	0.46
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.98	0.46
2:P:154:LEU:H	2:P:154:LEU:HD23	1.80	0.46
1:O:179:GLY:O	1:O:180:LEU:HD13	2.15	0.45
1:M:158:SER:O	1:M:159:TRP:HD1	1.99	0.45
1:Q:29:ILE:HD12	1:Q:30:ARG:N	2.31	0.45
1:O:48:TRP:HZ2	1:O:51:TYR:CD2	2.29	0.45
1:K:151:PHE:HA	1:K:152:PRO:HA	1.77	0.45
1:S:135:SER:HA	1:S:191:SER:OG	2.16	0.45
1:I:148:LYS:NZ	1:I:176:GLN:OE1	2.37	0.45
1:K:142:ALA:HB2	1:K:188:THR:HG22	1.99	0.45
1:A:29:ILE:HG23	1:A:35:TRP:NE1	2.31	0.45
1:A:53:HIS:HE1	1:A:54:TYR:CE2	2.34	0.45
1:K:30:ARG:O	1:K:54:TYR:HB2	2.16	0.45
1:G:173:ALA:HB2	1:G:183:LEU:HD23	1.97	0.45
2:D:39:LYS:HG2	2:D:84:ALA:HB2	1.98	0.45
2:L:78:LEU:HD11	2:L:106:ILE:HG12	1.98	0.45
1:M:100:ASP:OD1	1:M:101:SER:N	2.48	0.45
1:G:71:SER:O	1:G:80:SER:N	2.45	0.45
1:Q:27:TYR:HE1	1:Q:31:PHE:O	1.99	0.45
1:Q:29:ILE:HG13	1:Q:29:ILE:H	1.57	0.45
2:N:157:GLY:HA3	2:P:154:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.52	0.45
2:B:199:GLN:OE1	2:B:199:GLN:N	2.44	0.45
1:K:36:HIS:HD2	1:K:48:TRP:NE1	2.10	0.45
1:E:33:TYR:CD1	1:E:33:TYR:N	2.84	0.45
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.99	0.45
2:D:158:ASN:OD1	2:D:158:ASN:N	2.49	0.45
2:B:35:TRP:CG	2:B:73:LEU:HD12	2.52	0.45
2:P:108:ARG:NH1	2:P:142:ARG:H	2.14	0.45
2:R:33:LEU:HG	2:R:71:PHE:CG	2.52	0.45
2:D:35:TRP:CG	2:D:73:LEU:HD12	2.51	0.45
1:O:123:GLY:HA2	1:O:124:PRO:HD3	1.69	0.45
1:K:103:ASN:HB3	2:L:96:LEU:CD2	2.47	0.45
2:D:149:LYS:HG2	2:D:154:LEU:HD23	1.99	0.45
2:T:90:GLN:N	2:T:90:GLN:OE1	2.45	0.45
1:Q:18:LEU:N	1:Q:83:LEU:O	2.38	0.45
1:G:36:HIS:CD2	1:G:99:LYS:HB2	2.52	0.45
2:L:32:HIS:HD1	2:L:50:TYR:HE1	1.64	0.45
2:T:88:CYS:O	2:T:99:GLY:N	2.48	0.45
2:J:49:LYS:HG2	2:J:50:TYR:CD2	2.52	0.45
2:N:93:ASP:OD1	2:N:94:PHE:N	2.50	0.45
2:P:105:GLU:CG	2:P:106:ILE:H	2.30	0.45
1:K:28:PRO:HG2	1:K:31:PHE:CD2	2.52	0.45
1:O:171:PHE:HA	1:O:172:PRO:HD3	1.83	0.45
1:M:72:ARG:HA	1:M:79:PHE:HA	1.99	0.45
2:P:47:LEU:O	2:P:55:ILE:HG12	2.17	0.45
1:K:28:PRO:HG2	1:K:31:PHE:CG	2.52	0.45
2:N:33:LEU:HG	2:N:34:HIS:N	2.31	0.45
1:O:144:GLY:HA3	1:O:186:VAL:HG12	1.98	0.45
1:A:113:LEU:HD12	1:A:114:VAL:H	1.82	0.45
1:S:31:PHE:N	1:S:31:PHE:CD1	2.83	0.45
1:E:143:LEU:O	1:E:187:VAL:N	2.36	0.44
1:G:29:ILE:HG13	1:G:77:ASN:OD1	2.18	0.44
1:A:53:HIS:HB2	1:A:57:TYR:HB3	1.99	0.44
1:O:200:ILE:HG22	1:O:215:ARG:HA	1.99	0.44
1:A:168:VAL:HG22	1:A:187:VAL:HB	1.98	0.44
2:D:12:SER:HB3	2:F:10:PHE:HB3	1.99	0.44
1:E:34:SER:HB2	1:E:36:HIS:CE1	2.45	0.44
1:K:104:TYR:O	1:K:106:PRO:HD3	2.17	0.44
2:F:147:GLN:HB3	2:F:195:GLU:HB3	1.99	0.44
2:R:49:LYS:C	2:R:51:ALA:HA	2.37	0.44
1:A:27:TYR:OH	1:A:32:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:TYR:CD2	1:K:100:ASP:HA	2.52	0.44
2:J:61:ARG:HH22	2:J:79:GLU:HG3	1.82	0.44
2:D:158:ASN:HD22	2:D:181:LEU:HD21	1.82	0.44
1:I:104:TYR:O	1:I:106:PRO:HD3	2.17	0.44
2:L:88:CYS:O	2:L:99:GLY:N	2.49	0.44
2:H:112:ALA:HA	2:H:113:PRO:HD3	1.83	0.44
1:S:39:ARG:HD3	1:S:49:MET:HE3	2.00	0.44
1:A:48:TRP:HZ2	1:A:51:TYR:HD1	1.66	0.44
2:N:150:VAL:HG13	2:N:192:TYR:CE1	2.53	0.44
1:I:36:HIS:CD2	1:I:51:TYR:HB2	2.52	0.44
1:O:35:TRP:CG	1:O:79:PHE:CE1	3.06	0.44
2:R:210:ASN:OD1	2:R:210:ASN:N	2.51	0.44
2:R:55:ILE:HG22	2:R:56:SER:N	2.33	0.44
2:J:30:SER:O	2:J:32:HIS:N	2.44	0.44
1:O:52:ILE:HA	1:O:58:THR:HG22	2.00	0.44
1:S:71:SER:O	1:S:80:SER:N	2.36	0.44
2:J:188:LYS:HE2	2:J:188:LYS:HB3	1.83	0.44
1:S:131:PRO:HB3	1:S:143:LEU:HB3	2.00	0.44
2:B:46:LEU:O	2:B:55:ILE:HG21	2.18	0.44
2:T:49:LYS:C	2:T:51:ALA:HA	2.38	0.44
2:H:150:VAL:HG13	2:H:192:TYR:CE1	2.52	0.44
2:F:166:GLN:HE21	2:F:171:SER:HB3	1.83	0.44
2:P:35:TRP:CE2	2:P:73:LEU:HB2	2.52	0.44
1:Q:67:ARG:NH2	1:Q:86:VAL:HA	2.32	0.44
1:O:104:TYR:HB3	2:P:34:HIS:CE1	2.53	0.44
2:R:33:LEU:HD13	2:R:34:HIS:N	2.33	0.44
1:K:41:PRO:HB2	1:K:44:LYS:HB2	2.00	0.44
2:P:185:ASP:O	2:P:188:LYS:HG2	2.18	0.44
1:A:98:ARG:NH2	1:A:100:ASP:OD2	2.51	0.43
2:R:6:GLN:NE2	2:R:88:CYS:SG	2.90	0.43
2:T:23:CYS:HB2	2:T:35:TRP:CH2	2.53	0.43
1:I:29:ILE:HD11	1:I:77:ASN:C	2.39	0.43
1:E:164:LEU:HD11	1:E:187:VAL:HG21	1.99	0.43
1:E:54:TYR:HD1	1:E:55:SER:N	2.16	0.43
2:P:107:LYS:HD3	2:P:109:THR:CB	2.48	0.43
2:H:63:SER:O	2:H:73:LEU:HD12	2.18	0.43
1:E:204:ASN:HB2	1:E:211:LYS:HE2	1.99	0.43
2:T:78:LEU:HD11	2:T:106:ILE:HG12	2.01	0.43
1:Q:173:ALA:HB2	1:Q:183:LEU:HD23	2.00	0.43
1:G:29:ILE:HG22	1:G:35:TRP:NE1	2.32	0.43
2:P:7:SER:OG	2:P:22:THR:OG1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:LEU:HD22	2:H:89:GLN:O	2.18	0.43
1:O:192:SER:HA	1:Q:66:THR:HA	1.99	0.43
1:K:72:ARG:HA	1:K:79:PHE:HA	2.00	0.43
2:R:67:SER:OG	2:R:68:GLY:N	2.51	0.43
2:P:21:ILE:HG23	2:P:102:THR:HG21	2.00	0.43
1:O:27:TYR:HA	1:O:28:PRO:HD3	1.74	0.43
1:K:54:TYR:CD1	1:K:55:SER:N	2.87	0.43
1:I:18:LEU:N	1:I:83:LEU:O	2.42	0.43
2:L:33:LEU:HG	2:L:34:HIS:N	2.33	0.43
2:R:85:THR:HG22	2:R:103:LYS:HG3	2.00	0.43
2:N:33:LEU:HD12	2:N:89:GLN:O	2.18	0.43
1:C:33:TYR:N	1:C:33:TYR:CD2	2.85	0.43
2:T:142:ARG:HE	2:T:163:VAL:HG11	1.83	0.43
2:J:129:THR:HG23	1:Q:76:LYS:HE2	1.99	0.43
1:E:10:GLY:HA3	1:E:207:PRO:HG3	2.01	0.43
1:M:98:ARG:HH21	1:M:107:TYR:HE2	1.64	0.43
1:I:33:TYR:N	1:I:33:TYR:CD1	2.87	0.43
1:O:129:LEU:HB3	1:O:144:GLY:O	2.18	0.43
2:B:142:ARG:HE	2:B:163:VAL:HG11	1.84	0.43
2:B:112:ALA:HA	2:B:113:PRO:HD3	1.86	0.43
1:C:53:HIS:HB2	1:C:57:TYR:CB	2.49	0.43
2:J:145:LYS:HB3	2:J:197:THR:OG1	2.19	0.43
2:D:32:HIS:CE1	2:D:50:TYR:HE1	2.36	0.43
2:H:13:VAL:HG13	2:L:7:SER:HB2	2.01	0.43
1:O:168:VAL:HG13	1:O:187:VAL:HG22	2.00	0.43
2:B:39:LYS:HG2	2:B:84:ALA:HB2	2.01	0.43
1:M:36:HIS:HE2	1:M:99:LYS:HB2	1.77	0.43
2:F:21:ILE:HB	2:F:73:LEU:HB3	2.00	0.43
2:P:136:LEU:HB3	2:P:139:PHE:CE1	2.53	0.43
2:D:7:SER:HB2	2:F:13:VAL:HG13	2.00	0.43
2:F:36:TYR:HE1	2:F:89:GLN:CG	2.32	0.43
2:H:158:ASN:OD1	2:H:158:ASN:N	2.51	0.43
1:A:205:HIS:CD2	1:A:207:PRO:HD2	2.54	0.43
1:Q:173:ALA:HA	1:Q:183:LEU:HB3	2.01	0.43
2:T:32:HIS:HB3	2:T:91:GLY:HA3	2.01	0.43
2:J:155:GLN:OE1	2:J:158:ASN:ND2	2.41	0.43
1:C:64:LEU:O	1:C:67:ARG:N	2.52	0.43
1:G:61:ASN:HA	1:G:62:PRO:HD3	1.92	0.43
1:S:48:TRP:HZ2	1:S:51:TYR:HD2	1.66	0.43
1:C:37:TRP:HB3	1:C:49:MET:HE3	2.00	0.43
1:A:8:GLY:HA3	1:A:20:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:LEU:O	2:J:34:HIS:ND1	2.52	0.42
1:Q:61:ASN:CG	1:Q:62:PRO:HD2	2.38	0.42
2:J:7:SER:OG	2:J:22:THR:OG1	2.28	0.42
2:J:25:ALA:O	2:J:69:THR:HG23	2.19	0.42
1:O:61:ASN:HA	1:O:62:PRO:HD3	1.86	0.42
2:R:166:GLN:HE21	2:R:171:SER:HB3	1.83	0.42
2:L:19:VAL:HB	2:L:75:ILE:HB	2.01	0.42
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.89	0.42
2:D:60:SER:O	2:R:24:ARG:NH1	2.35	0.42
2:H:23:CYS:HB2	2:H:35:TRP:CH2	2.54	0.42
2:P:147:GLN:HB3	2:P:195:GLU:HB2	2.00	0.42
1:O:29:ILE:N	1:O:29:ILE:HD13	2.34	0.42
2:N:88:CYS:O	2:N:99:GLY:N	2.53	0.42
2:P:35:TRP:CZ3	2:P:88:CYS:HB3	2.55	0.42
1:M:151:PHE:HA	1:M:152:PRO:HA	1.81	0.42
2:J:29:ILE:HD13	2:J:90:GLN:HB3	2.00	0.42
2:P:121:SER:O	2:P:124:GLN:HG2	2.19	0.42
2:P:123:GLU:O	2:P:126:LYS:HG2	2.19	0.42
2:L:59:PRO:HG2	2:L:62:PHE:HD2	1.85	0.42
2:F:63:SER:OG	2:F:64:GLY:N	2.52	0.42
1:E:32:GLY:O	1:E:54:TYR:CD2	2.73	0.42
2:F:21:ILE:HG23	2:F:102:THR:HG21	2.01	0.42
1:I:54:TYR:O	1:I:72:ARG:NH2	2.45	0.42
1:A:201:CYS:SG	1:A:214:LYS:HB2	2.59	0.42
2:F:150:VAL:HG13	2:F:192:TYR:CE1	2.55	0.42
1:G:36:HIS:HE2	1:G:99:LYS:HB2	1.82	0.42
2:R:55:ILE:HG22	2:R:56:SER:H	1.85	0.42
2:L:49:LYS:HG2	2:L:50:TYR:CD2	2.51	0.42
1:I:98:ARG:NH1	1:I:100:ASP:HA	2.35	0.42
1:A:191:SER:HA	1:A:194:LEU:HD13	2.02	0.42
1:I:206:LYS:HD2	1:I:206:LYS:HA	1.86	0.42
1:M:205:HIS:ND1	1:M:208:SER:HB3	2.34	0.42
2:H:2:ILE:O	2:H:97:THR:HG21	2.20	0.42
1:M:54:TYR:CD1	1:M:55:SER:N	2.82	0.42
1:S:122:LYS:HB3	1:S:123:GLY:HA3	2.01	0.42
2:D:33:LEU:HD13	2:D:34:HIS:N	2.34	0.42
2:H:150:VAL:HG13	2:H:192:TYR:HE1	1.85	0.42
1:C:149:ASP:HA	1:C:180:LEU:HB3	2.02	0.42
1:Q:124:PRO:HB3	1:Q:150:TYR:HB3	2.00	0.42
2:H:125:LEU:HD13	2:H:125:LEU:HA	1.93	0.42
1:G:31:PHE:CD1	1:G:31:PHE:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:HIS:HB2	2:D:89:GLN:HG3	2.02	0.42
2:R:36:TYR:CE1	2:R:89:GLN:HG2	2.54	0.42
1:S:104:TYR:HB3	2:T:34:HIS:CD2	2.55	0.42
2:B:35:TRP:CD2	2:B:73:LEU:HD12	2.54	0.42
1:A:143:LEU:HB2	1:A:216:VAL:HG11	2.01	0.42
1:A:190:PRO:O	1:A:193:SER:OG	2.27	0.42
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.55	0.42
1:C:122:LYS:HD2	1:C:149:ASP:O	2.18	0.42
2:L:192:TYR:HB2	2:L:209:PHE:CE1	2.55	0.42
1:K:60:PHE:HE1	1:K:70:ILE:HG13	1.84	0.42
2:L:2:ILE:O	2:L:97:THR:HG21	2.19	0.42
1:Q:67:ARG:HH22	1:Q:86:VAL:HA	1.85	0.42
2:B:13:VAL:HG21	2:B:19:VAL:HG22	2.01	0.42
2:R:29:ILE:HB	2:R:71:PHE:HE2	1.85	0.42
1:O:151:PHE:HA	1:O:152:PRO:HA	1.82	0.42
2:H:89:GLN:HG2	2:H:90:GLN:N	2.34	0.41
2:L:61:ARG:NH1	2:L:79:GLU:HB2	2.35	0.41
2:J:14:THR:OG1	2:J:17:GLU:HG3	2.20	0.41
1:K:31:PHE:N	1:K:31:PHE:HD1	2.17	0.41
2:J:108:ARG:HG2	2:J:140:TYR:CD2	2.55	0.41
1:A:151:PHE:HA	1:A:152:PRO:HA	1.83	0.41
1:E:60:PHE:O	1:E:65:LYS:NZ	2.53	0.41
2:D:18:LYS:HB3	2:D:18:LYS:HE2	1.81	0.41
1:Q:62:PRO:HD3	2:R:95:PRO:CG	2.50	0.41
2:N:47:LEU:HD23	2:N:47:LEU:HA	1.93	0.41
2:R:6:GLN:HE21	2:R:99:GLY:HA3	1.86	0.41
2:N:17:GLU:OE2	2:P:24:ARG:NH2	2.28	0.41
1:E:54:TYR:CD1	1:E:55:SER:N	2.88	0.41
1:I:124:PRO:CB	1:I:150:TYR:HB3	2.45	0.41
2:L:24:ARG:HG2	2:L:69:THR:HG22	2.01	0.41
2:T:175:LEU:HD23	2:T:176:SER:N	2.35	0.41
2:R:29:ILE:O	2:R:29:ILE:HG22	2.20	0.41
1:C:123:GLY:HA2	1:C:124:PRO:HD3	1.84	0.41
1:K:106:PRO:HG2	1:K:107:TYR:CD2	2.55	0.41
1:G:32:GLY:O	1:G:54:TYR:CD2	2.73	0.41
1:K:100:ASP:OD1	1:K:101:SER:N	2.50	0.41
2:H:140:TYR:CG	2:H:141:PRO:HA	2.55	0.41
2:H:124:GLN:HG2	2:H:129:THR:O	2.20	0.41
2:F:134:CYS:HB2	2:F:148:TRP:CH2	2.56	0.41
1:A:122:LYS:O	1:A:205:HIS:HE1	2.04	0.41
1:O:104:TYR:O	1:O:106:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:ASP:OD1	1:I:101:SER:N	2.49	0.41
1:Q:104:TYR:HB3	2:R:34:HIS:NE2	2.35	0.41
2:H:157:GLY:HA3	2:L:154:LEU:HD13	2.03	0.41
1:K:134:LYS:HB3	1:K:137:SER:HB2	2.02	0.41
1:I:29:ILE:HG23	1:I:35:TRP:NE1	2.36	0.41
1:K:6:GLU:CD	1:K:111:GLY:H	2.22	0.41
2:H:47:LEU:HA	2:H:47:LEU:HD23	1.94	0.41
1:E:51:TYR:CE2	2:F:94:PHE:HE2	2.39	0.41
1:O:176:GLN:HG2	1:O:179:GLY:H	1.86	0.41
1:K:104:TYR:CZ	2:L:49:LYS:HE2	2.56	0.41
1:C:173:ALA:HA	1:C:183:LEU:HB3	2.02	0.41
1:G:104:TYR:O	1:G:106:PRO:HD3	2.21	0.41
2:D:35:TRP:CD2	2:D:73:LEU:HD12	2.56	0.41
1:E:104:TYR:O	1:E:106:PRO:HD3	2.21	0.41
1:E:48:TRP:CE3	1:E:61:ASN:HB2	2.56	0.41
1:G:18:LEU:HB3	1:G:83:LEU:HB3	2.03	0.41
2:J:34:HIS:ND1	2:J:49:LYS:HG3	2.36	0.41
1:K:48:TRP:CZ2	1:K:50:GLY:HA2	2.56	0.41
2:F:134:CYS:HB2	2:F:148:TRP:CZ2	2.54	0.41
1:I:168:VAL:HG12	1:I:187:VAL:HB	2.02	0.41
1:O:20:LEU:HB2	1:O:81:LEU:CD2	2.50	0.41
1:O:81:LEU:O	1:O:82:LYS:HG2	2.20	0.41
2:L:49:LYS:HZ2	2:L:50:TYR:HE2	1.67	0.41
2:D:47:LEU:O	2:D:55:ILE:HG12	2.21	0.41
1:M:48:TRP:CE3	1:M:61:ASN:HB2	2.56	0.41
2:N:7:SER:HG	2:N:22:THR:HG1	1.62	0.41
2:F:33:LEU:HG	2:F:71:PHE:CG	2.56	0.41
1:S:34:SER:HB2	1:S:53:HIS:HA	2.02	0.41
1:G:65:LYS:HE3	1:G:65:LYS:HB2	1.86	0.41
2:T:29:ILE:HG22	2:T:92:TYR:HD2	1.85	0.41
1:Q:217:GLU:HA	1:Q:218:PRO:HD3	1.92	0.41
2:N:158:ASN:OD1	2:N:158:ASN:N	2.54	0.41
1:G:212:VAL:HA	1:Q:211:LYS:O	2.21	0.41
1:E:129:LEU:HD11	2:F:118:PHE:CG	2.56	0.41
2:N:90:GLN:OE1	2:N:92:TYR:N	2.54	0.41
1:A:29:ILE:HG23	1:A:35:TRP:CD1	2.55	0.41
1:A:32:GLY:O	1:A:54:TYR:HB3	2.21	0.41
2:D:107:LYS:HD3	2:F:9:ASP:OD2	2.21	0.41
1:E:146:LEU:HD12	1:E:183:LEU:O	2.21	0.41
2:T:210:ASN:HB3	2:T:211:ARG:H	1.78	0.41
2:F:35:TRP:CE2	2:F:73:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:104:TYR:O	1:M:106:PRO:HD3	2.21	0.40
1:Q:104:TYR:HB3	2:R:34:HIS:CE1	2.55	0.40
1:S:29:ILE:HG13	1:S:29:ILE:H	1.75	0.40
1:O:35:TRP:CG	1:O:79:PHE:HE1	2.39	0.40
1:I:53:HIS:CB	1:I:57:TYR:HB3	2.51	0.40
2:N:89:GLN:O	2:N:89:GLN:HG3	2.21	0.40
1:Q:63:SER:C	1:Q:64:LEU:HG	2.42	0.40
2:P:105:GLU:CG	2:P:106:ILE:N	2.84	0.40
2:P:192:TYR:HB2	2:P:209:PHE:CE1	2.55	0.40
2:L:4:LEU:HD12	2:L:23:CYS:SG	2.62	0.40
1:E:146:LEU:HD21	1:E:148:LYS:NZ	2.36	0.40
1:I:71:SER:O	1:I:80:SER:N	2.50	0.40
2:N:149:LYS:HG2	2:N:154:LEU:HD23	2.04	0.40
2:J:33:LEU:HD22	2:J:34:HIS:H	1.85	0.40
1:C:104:TYR:HB3	2:D:34:HIS:CE1	2.56	0.40
2:P:136:LEU:HD22	2:P:139:PHE:HE1	1.86	0.40
2:N:37:GLN:HB2	2:N:47:LEU:HD11	2.02	0.40
1:S:191:SER:HA	1:S:194:LEU:HD13	2.03	0.40
1:A:18:LEU:N	1:A:83:LEU:O	2.41	0.40
1:O:64:LEU:H	1:O:64:LEU:HG	1.63	0.40
2:N:13:VAL:HG13	2:P:7:SER:HB2	2.03	0.40
1:E:33:TYR:HB2	1:E:98:ARG:HD2	2.04	0.40
2:J:4:LEU:HD12	2:J:23:CYS:SG	2.62	0.40
1:K:53:HIS:HD2	1:K:57:TYR:CD2	2.40	0.40
1:Q:104:TYR:HB3	2:R:34:HIS:CD2	2.56	0.40
2:R:33:LEU:HG	2:R:71:PHE:CD2	2.56	0.40
2:H:149:LYS:HG2	2:H:154:LEU:HD23	2.04	0.40
2:T:39:LYS:HG2	2:T:84:ALA:HB2	2.03	0.40
2:R:39:LYS:HG2	2:R:84:ALA:HB2	2.04	0.40
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.88	0.40
1:M:31:PHE:N	1:M:31:PHE:CD1	2.89	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	216/225 (96%)	206 (95%)	9 (4%)	1 (0%)	34	77
1	C	216/225 (96%)	206 (95%)	10 (5%)	0	100	100
1	E	216/225 (96%)	209 (97%)	6 (3%)	1 (0%)	34	77
1	G	216/225 (96%)	210 (97%)	5 (2%)	1 (0%)	34	77
1	I	216/225 (96%)	207 (96%)	9 (4%)	0	100	100
1	K	216/225 (96%)	209 (97%)	6 (3%)	1 (0%)	34	77
1	M	216/225 (96%)	210 (97%)	6 (3%)	0	100	100
1	O	216/225 (96%)	207 (96%)	8 (4%)	1 (0%)	34	77
1	Q	216/225 (96%)	207 (96%)	8 (4%)	1 (0%)	34	77
1	S	216/225 (96%)	206 (95%)	9 (4%)	1 (0%)	34	77
2	B	209/214 (98%)	201 (96%)	7 (3%)	1 (0%)	34	77
2	D	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	F	209/214 (98%)	204 (98%)	5 (2%)	0	100	100
2	H	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	J	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
2	L	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	N	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
2	P	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
2	R	211/214 (99%)	196 (93%)	15 (7%)	0	100	100
2	T	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
All	All	4252/4390 (97%)	4086 (96%)	158 (4%)	8 (0%)	52	87

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	E	209	ASN
1	G	33	TYR
2	B	137	ASN
1	K	65	LYS
1	S	207	PRO
1	Q	56	GLY
1	O	28	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	189/196 (96%)	180 (95%)	9 (5%)	31	71
1	C	189/196 (96%)	179 (95%)	10 (5%)	28	67
1	E	189/196 (96%)	181 (96%)	8 (4%)	36	74
1	G	189/196 (96%)	184 (97%)	5 (3%)	54	83
1	I	189/196 (96%)	181 (96%)	8 (4%)	36	74
1	K	189/196 (96%)	181 (96%)	8 (4%)	36	74
1	M	189/196 (96%)	185 (98%)	4 (2%)	61	86
1	O	189/196 (96%)	173 (92%)	16 (8%)	13	49
1	Q	189/196 (96%)	185 (98%)	4 (2%)	61	86
1	S	189/196 (96%)	181 (96%)	8 (4%)	36	74
2	B	187/189 (99%)	181 (97%)	6 (3%)	46	80
2	D	187/189 (99%)	184 (98%)	3 (2%)	70	89
2	F	187/189 (99%)	184 (98%)	3 (2%)	70	89
2	H	187/189 (99%)	182 (97%)	5 (3%)	52	83
2	J	187/189 (99%)	180 (96%)	7 (4%)	41	76
2	L	187/189 (99%)	183 (98%)	4 (2%)	61	86
2	N	187/189 (99%)	183 (98%)	4 (2%)	61	86
2	P	187/189 (99%)	176 (94%)	11 (6%)	24	64
2	R	188/189 (100%)	182 (97%)	6 (3%)	46	80
2	T	187/189 (99%)	181 (97%)	6 (3%)	46	80
All	All	3761/3850 (98%)	3626 (96%)	135 (4%)	42	77

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	27	TYR
1	A	31	PHE

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Mol	Chain	Res	Type
1	A	33	TYR
1	A	64	LEU
1	A	115	THR
1	A	122	LYS
1	A	143	LEU
1	A	187	VAL
2	B	28	SER
2	B	32	HIS
2	B	50	TYR
2	B	53	HIS
2	B	92	TYR
2	B	137	ASN
1	C	30	ARG
1	C	51	TYR
1	C	53	HIS
1	C	54	TYR
1	C	55	SER
1	C	57	TYR
1	C	64	LEU
1	C	66	THR
1	C	83	LEU
1	C	164	LEU
2	D	30	SER
2	D	31	ASP
2	D	52	SER
1	E	30	ARG
1	E	31	PHE
1	E	34	SER
1	E	54	TYR
1	E	55	SER
1	E	57	TYR
1	E	110	GLN
1	E	197	GLN
2	F	27	GLN
2	F	31	ASP
2	F	109	THR
1	G	29	ILE
1	G	31	PHE
1	G	33	TYR
1	G	54	TYR
1	G	55	SER
2	H	50	TYR

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Mol	Chain	Res	Type
2	H	90	GLN
2	H	92	TYR
2	H	108	ARG
2	H	147	GLN
1	I	30	ARG
1	I	51	TYR
1	I	53	HIS
1	I	54	TYR
1	I	58	THR
1	I	81	LEU
1	I	121	THR
1	I	122	LYS
2	J	31	ASP
2	J	48	ILE
2	J	61	ARG
2	J	89	GLN
2	J	90	GLN
2	J	97	THR
2	J	109	THR
1	K	31	PHE
1	K	33	TYR
1	K	34	SER
1	K	53	HIS
1	K	54	TYR
1	K	98	ARG
1	K	104	TYR
1	K	120	SER
2	L	9	ASP
2	L	26	SER
2	L	96	LEU
2	L	109	THR
1	M	54	TYR
1	M	201	CYS
1	M	202	ASN
1	M	209	ASN
2	N	32	HIS
2	N	50	TYR
2	N	61	ARG
2	N	89	GLN
1	O	18	LEU
1	O	29	ILE
1	O	30	ARG

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Mol	Chain	Res	Type
1	O	33	TYR
1	O	55	SER
1	O	64	LEU
1	O	72	ARG
1	O	77	ASN
1	O	81	LEU
1	O	122	LYS
1	O	129	LEU
1	O	143	LEU
1	O	159	TRP
1	O	180	LEU
1	O	183	LEU
1	O	189	VAL
2	P	48	ILE
2	P	49	LYS
2	P	50	TYR
2	P	106	ILE
2	P	108	ARG
2	P	115	VAL
2	P	117	ILE
2	P	139	PHE
2	P	140	TYR
2	P	183	LYS
2	P	186	TYR
1	Q	29	ILE
1	Q	57	TYR
1	Q	63	SER
1	Q	64	LEU
2	R	69	THR
2	R	70	ASP
2	R	92	TYR
2	R	96	LEU
2	R	209	PHE
2	R	210	ASN
1	S	31	PHE
1	S	53	HIS
1	S	60	PHE
1	S	63	SER
1	S	64	LEU
1	S	66	THR
1	S	67	ARG
1	S	69	THR

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Mol	Chain	Res	Type
2	T	47	LEU
2	T	89	GLN
2	T	92	TYR
2	T	109	THR
2	T	136	LEU
2	T	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	ASN
1	E	36	HIS
1	G	204	ASN
2	H	124	GLN
2	J	34	HIS
2	J	89	GLN
1	K	36	HIS
1	K	53	HIS
1	M	160	ASN
2	N	124	GLN
1	O	53	HIS
2	P	34	HIS
2	P	166	GLN
2	R	89	GLN
1	S	169	HIS
2	T	6	GLN
2	T	89	GLN
2	T	124	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	218/225 (96%)	0.03	2 (0%) 85 79	78, 111, 160, 222	0
1	C	218/225 (96%)	0.14	7 (3%) 51 45	91, 122, 177, 248	0
1	E	218/225 (96%)	0.46	14 (6%) 23 21	102, 159, 254, 334	0
1	G	218/225 (96%)	0.18	2 (0%) 85 79	84, 110, 166, 227	0
1	I	218/225 (96%)	0.32	9 (4%) 41 35	105, 141, 197, 248	0
1	K	218/225 (96%)	0.25	6 (2%) 56 50	111, 146, 197, 255	0
1	M	218/225 (96%)	0.19	7 (3%) 51 45	86, 120, 200, 273	0
1	O	218/225 (96%)	1.03	45 (20%) 1 1	120, 192, 301, 337	0
1	Q	218/225 (96%)	0.24	7 (3%) 51 45	102, 138, 186, 228	0
1	S	218/225 (96%)	0.88	31 (14%) 4 4	156, 224, 263, 304	0
2	B	211/214 (98%)	0.08	0 100 100	86, 120, 146, 170	0
2	D	211/214 (98%)	-0.02	0 100 100	78, 123, 156, 173	0
2	F	211/214 (98%)	0.09	1 (0%) 91 89	97, 139, 197, 224	0
2	H	211/214 (98%)	0.05	3 (1%) 78 71	92, 122, 148, 171	0
2	J	211/214 (98%)	-0.04	0 100 100	95, 131, 160, 193	0
2	L	211/214 (98%)	-0.01	3 (1%) 78 71	101, 133, 164, 184	0
2	N	211/214 (98%)	0.01	1 (0%) 91 89	96, 142, 204, 251	0
2	P	211/214 (98%)	0.95	30 (14%) 4 4	109, 191, 319, 344	0
2	R	213/214 (99%)	0.47	11 (5%) 31 27	109, 152, 202, 223	0
2	T	211/214 (98%)	1.99	90 (42%) 0 0	186, 255, 312, 338	0
All	All	4292/4390 (97%)	0.36	269 (6%) 23 21	78, 139, 262, 344	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	181	LEU	17.2
1	S	136	THR	13.0
1	O	131	PRO	13.0
1	E	136	THR	9.7
2	P	149	LYS	9.6
1	O	189	VAL	8.7
2	P	191	VAL	8.5
2	P	206	THR	8.4
1	O	165	THR	7.9
2	T	104	VAL	7.7
1	O	188	THR	7.1
2	T	2	ILE	7.0
2	P	151	ASP	7.0
1	E	137	SER	6.9
1	S	83	LEU	6.6
2	T	29	ILE	6.6
1	E	135	SER	6.5
2	T	194	CYS	6.4
2	T	11	GLN	6.2
2	T	148	TRP	5.9
2	P	180	THR	5.9
1	Q	136	THR	5.9
2	P	122	ASP	5.9
1	O	190	PRO	5.8
1	O	193	SER	5.7
2	T	159	SER	5.6
1	C	135	SER	5.6
1	O	145	CYS	5.5
2	T	28	SER	5.5
1	O	164	LEU	5.4
2	P	153	ALA	5.4
1	Q	135	SER	5.4
2	P	121	SER	5.4
2	T	191	VAL	5.3
2	T	149	LYS	5.3
1	Q	137	SER	5.2
2	T	207	LYS	5.2
2	T	190	LYS	5.2
2	T	75	ILE	5.1
2	T	200	GLY	5.1
2	P	208	SER	5.1
1	I	136	THR	5.0
1	O	199	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
2	P	207	LYS	5.0
2	P	190	LYS	5.0
1	O	162	GLY	5.0
2	P	154	LEU	5.0
2	T	78	LEU	4.9
1	O	163	ALA	4.8
1	O	126	VAL	4.8
1	S	82	LYS	4.6
2	T	77	SER	4.6
1	I	135	SER	4.6
1	S	137	SER	4.6
2	T	186	TYR	4.6
1	M	136	THR	4.6
2	T	193	ALA	4.5
2	T	96	LEU	4.5
1	O	159	TRP	4.5
2	T	147	GLN	4.5
2	T	19	VAL	4.5
2	P	130	ALA	4.4
2	T	30	SER	4.4
2	T	15	PRO	4.3
1	O	161	SER	4.3
1	S	138	GLY	4.3
1	A	135	SER	4.2
2	T	204	PRO	4.2
1	O	132	SER	4.2
1	S	135	SER	4.2
1	O	213	ASP	4.1
2	T	8	PRO	4.0
1	E	194	LEU	3.9
1	O	194	LEU	3.9
1	A	136	THR	3.9
2	T	59	PRO	3.9
1	C	137	SER	3.9
1	O	200	ILE	3.9
1	O	218	PRO	3.8
2	T	92	TYR	3.8
1	E	128	PRO	3.8
2	L	181	LEU	3.7
2	T	98	PHE	3.7
2	T	137	ASN	3.7
2	T	54	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	135	SER	3.7
2	R	147	GLN	3.7
2	T	189	HIS	3.7
1	O	166	SER	3.6
2	T	208	SER	3.6
2	T	177	SER	3.6
1	C	136	THR	3.6
2	T	205	VAL	3.6
1	E	138	GLY	3.6
1	O	150	TYR	3.5
1	S	114	VAL	3.5
2	T	196	VAL	3.5
1	S	185	SER	3.5
2	T	155	GLN	3.5
2	T	48	ILE	3.5
2	P	196	VAL	3.5
1	K	135	SER	3.5
2	T	64	GLY	3.4
1	E	199	TYR	3.4
2	T	107	LYS	3.4
1	O	136	THR	3.4
1	O	138	GLY	3.4
2	T	97	THR	3.4
2	P	139	PHE	3.4
2	P	197	THR	3.4
1	O	130	ALA	3.4
2	T	106	ILE	3.3
1	S	46	LEU	3.3
1	O	191	SER	3.3
2	R	148	TRP	3.2
1	O	143	LEU	3.2
2	F	126	LYS	3.2
2	T	150	VAL	3.2
1	O	196	THR	3.2
2	P	144	ALA	3.2
2	T	158	ASN	3.1
2	T	87	TYR	3.1
1	S	38	ILE	3.1
2	R	35	TRP	3.1
1	K	199	TYR	3.1
2	T	151	ASP	3.1
1	S	171	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	P	182	SER	3.1
2	T	103	LYS	3.1
2	R	6	GLN	3.0
1	O	181	TYR	3.0
1	S	18	LEU	3.0
2	T	188	LYS	3.0
1	E	115	THR	3.0
1	I	199	TYR	3.0
2	T	110	VAL	3.0
2	P	135	LEU	3.0
2	T	38	GLN	3.0
2	T	102	THR	3.0
1	O	160	ASN	3.0
2	R	29	ILE	2.9
1	O	147	VAL	2.9
2	T	162	SER	2.9
2	T	58	VAL	2.9
1	E	190	PRO	2.9
1	S	49	MET	2.9
1	M	141	ALA	2.9
2	T	135	LEU	2.8
1	I	130	ALA	2.8
1	I	138	GLY	2.8
1	I	145	CYS	2.8
1	G	135	SER	2.8
2	P	120	PRO	2.8
2	T	7	SER	2.8
1	E	130	ALA	2.8
1	S	80	SER	2.8
2	T	203	SER	2.8
1	K	136	THR	2.8
2	T	16	LYS	2.7
2	L	115	VAL	2.7
1	G	136	THR	2.7
2	T	198	HIS	2.7
2	T	91	GLY	2.7
1	O	185	SER	2.7
2	P	150	VAL	2.7
2	T	99	GLY	2.7
1	K	216	VAL	2.7
2	T	36	TYR	2.7
1	O	216	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	199	GLN	2.7
2	T	6	GLN	2.7
2	P	133	VAL	2.7
1	O	137	SER	2.7
2	T	71	PHE	2.7
1	S	149	ASP	2.6
2	T	185	ASP	2.6
1	S	180	LEU	2.6
2	H	193	ALA	2.6
1	Q	105	PHE	2.6
2	P	108	ARG	2.6
2	T	210	ASN	2.6
2	T	94	PHE	2.6
1	S	108	TRP	2.6
1	S	184	SER	2.6
1	Q	138	GLY	2.6
1	I	143	LEU	2.6
1	S	112	THR	2.6
2	L	130	ALA	2.5
2	T	27	GLN	2.5
1	E	150	TYR	2.5
1	C	138	GLY	2.5
1	S	85	SER	2.5
2	T	26	SER	2.5
1	Q	83	LEU	2.5
2	T	37	GLN	2.5
2	P	192	TYR	2.5
1	O	184	SER	2.5
2	R	78	LEU	2.5
2	T	206	THR	2.5
1	S	19	SER	2.5
2	T	76	ASN	2.5
1	O	144	GLY	2.5
2	T	201	LEU	2.4
2	T	4	LEU	2.4
2	R	47	LEU	2.4
1	O	128	PRO	2.4
2	T	154	LEU	2.4
2	R	192	TYR	2.4
2	T	195	GLU	2.4
1	S	169	HIS	2.4
2	T	192	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	187	VAL	2.4
2	T	199	GLN	2.4
1	M	199	TYR	2.4
1	O	198	THR	2.4
2	T	60	SER	2.4
2	H	192	TYR	2.3
2	T	21	ILE	2.3
2	T	142	ARG	2.3
1	S	78	GLN	2.3
2	P	112	ALA	2.3
2	T	174	SER	2.3
1	E	196	THR	2.3
2	T	100	GLY	2.3
1	M	143	LEU	2.3
2	T	161	GLU	2.3
2	T	140	TYR	2.3
1	O	152	PRO	2.3
1	I	137	SER	2.3
1	O	135	SER	2.3
2	T	53	HIS	2.3
2	T	163	VAL	2.3
1	S	167	GLY	2.2
2	H	96	LEU	2.2
1	K	159	TRP	2.2
2	T	3	VAL	2.2
2	T	160	GLN	2.2
2	P	148	TRP	2.2
2	T	143	GLU	2.2
2	T	187	GLU	2.2
1	S	152	PRO	2.2
1	C	143	LEU	2.2
1	O	212	VAL	2.2
1	S	84	SER	2.2
1	O	60	PHE	2.2
2	T	81	GLU	2.2
1	C	132	SER	2.2
2	P	152	ASN	2.2
1	O	158	SER	2.2
2	R	193	ALA	2.1
1	Q	47	GLU	2.1
1	O	133	SER	2.1
1	M	142	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	68	ILE	2.1
1	I	194	LEU	2.1
1	O	203	VAL	2.1
1	S	90	ASP	2.1
2	P	193	ALA	2.1
1	C	194	LEU	2.1
1	M	132	SER	2.1
1	E	134	LYS	2.1
2	R	53	HIS	2.1
1	S	77	ASN	2.0
2	N	148	TRP	2.0
1	K	184	SER	2.0
1	S	115	THR	2.0
1	E	12	VAL	2.0
2	R	65	SER	2.0
1	S	139	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.