Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 03:00 am BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

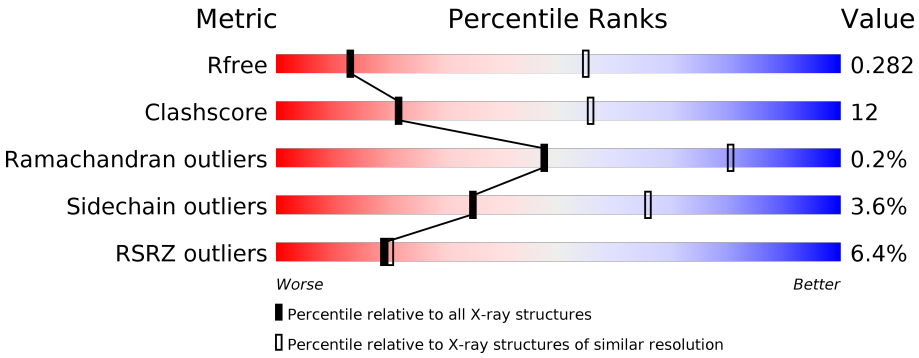
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	% 69% 25%
1	C	225	3% 74% 20%
1	E	225	7% 69% 26%
1	G	225	% 75% 20%
1	I	225	4% 76% 20%
1	K	225	3% 74% 20%

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Mol	Chain	Length	Quality of chain
1	M	225	3% 77% 19%
1	O	225	20% 62% 29% 6%
1	Q	225	3% 73% 23%
1	S	225	14% 68% 26%
2	B	214	76% 21%
2	D	214	79% 20%
2	F	214	73% 25%
2	H	214	% 75% 22%
2	J	214	75% 21%
2	L	214	% 69% 28%
2	N	214	78% 20%
2	P	214	14% 66% 29%
2	R	214	5% 72% 25%
2	T	214	44% 75% 21%

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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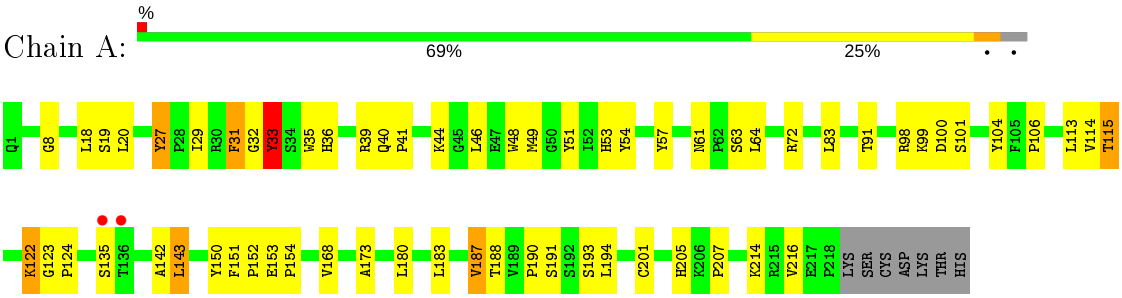
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	L	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	N	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	P	211	Total	C	N	O	S	0	0	0
			1635	1027	273	331	4			
2	R	213	Total	C	N	O	S	0	0	0
			1648	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

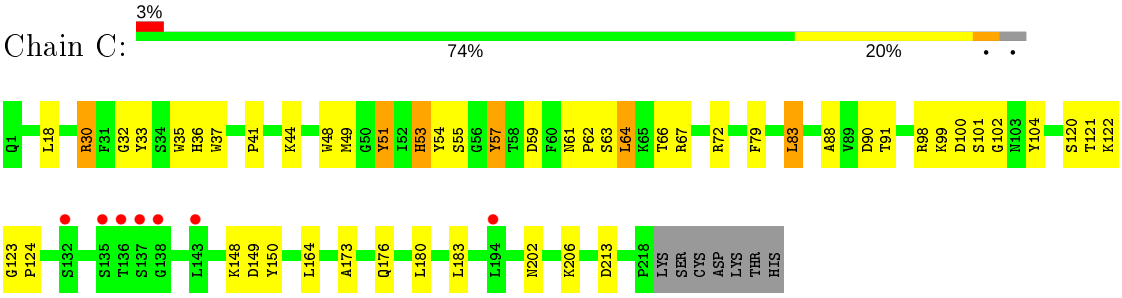
- Molecule 1: Fab C2E3 Heavy chain

Chain A:



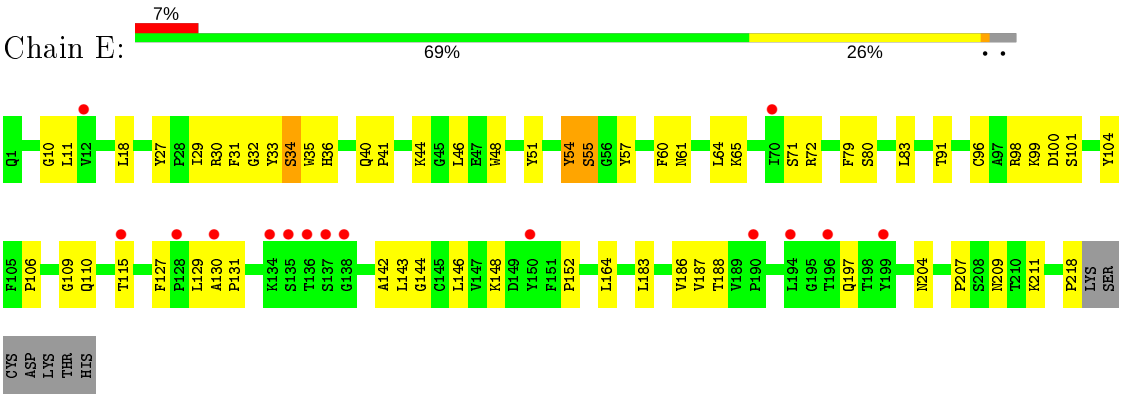
- Molecule 1: Fab C2E3 Heavy chain

Chain C:



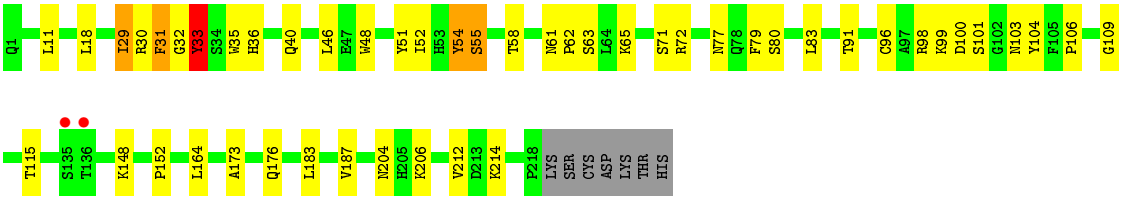
- Molecule 1: Fab C2E3 Heavy chain

Chain E:

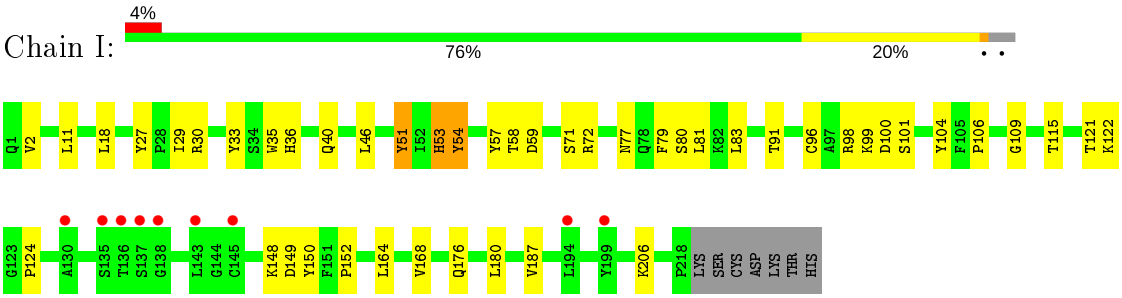


- Molecule 1: Fab C2E3 Heavy chain

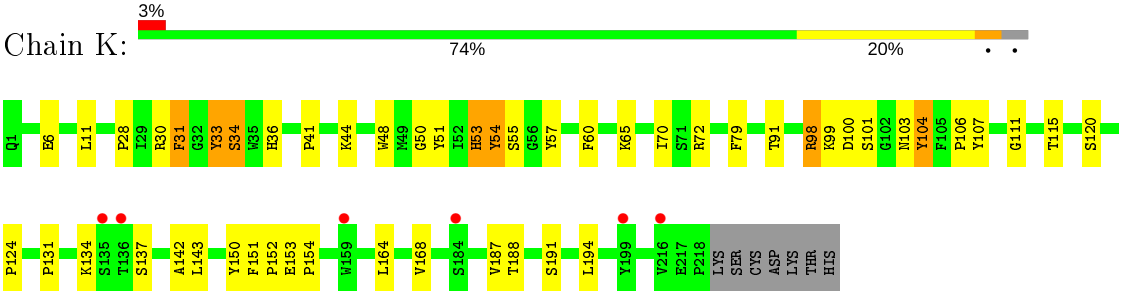
Chain G:



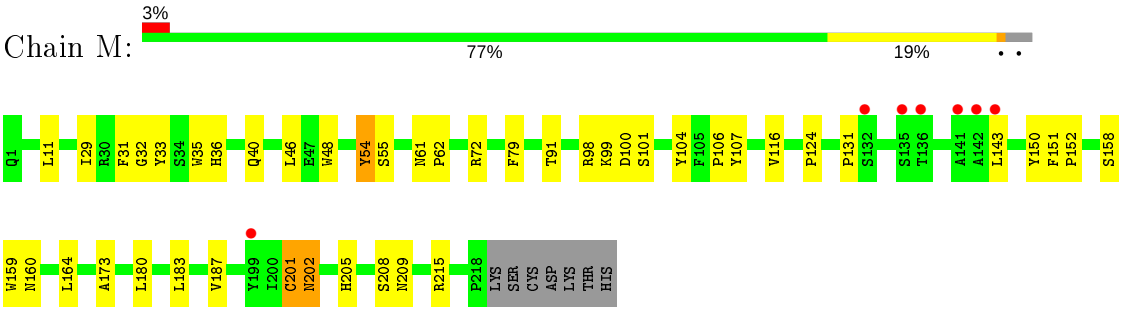
• Molecule 1: Fab C2E3 Heavy chain



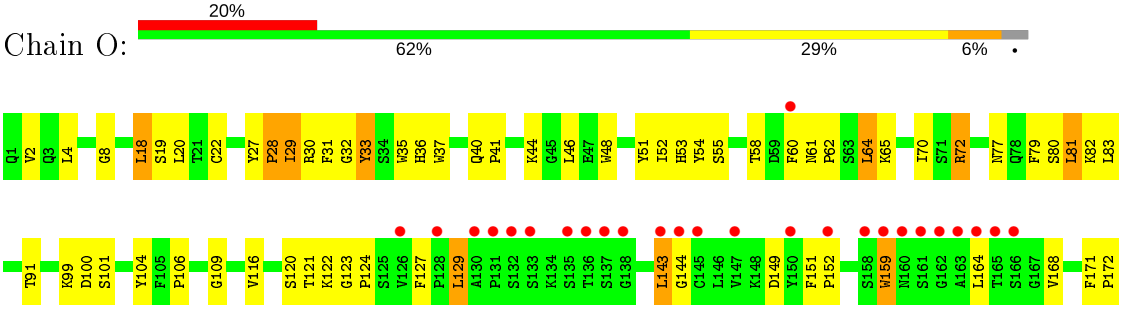
• Molecule 1: Fab C2E3 Heavy chain

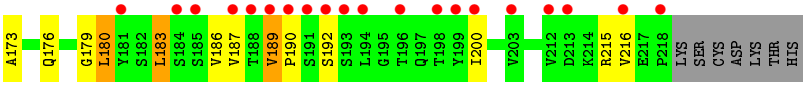


• Molecule 1: Fab C2E3 Heavy chain



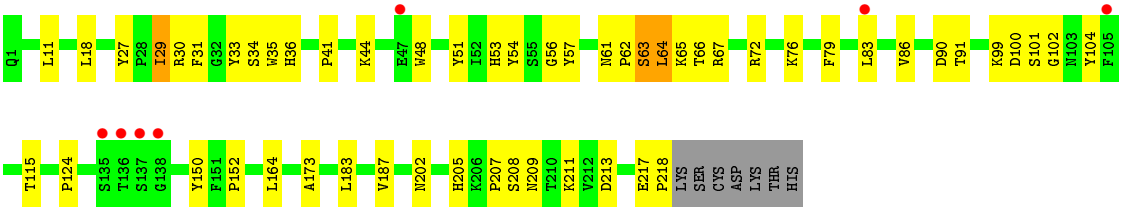
• Molecule 1: Fab C2E3 Heavy chain





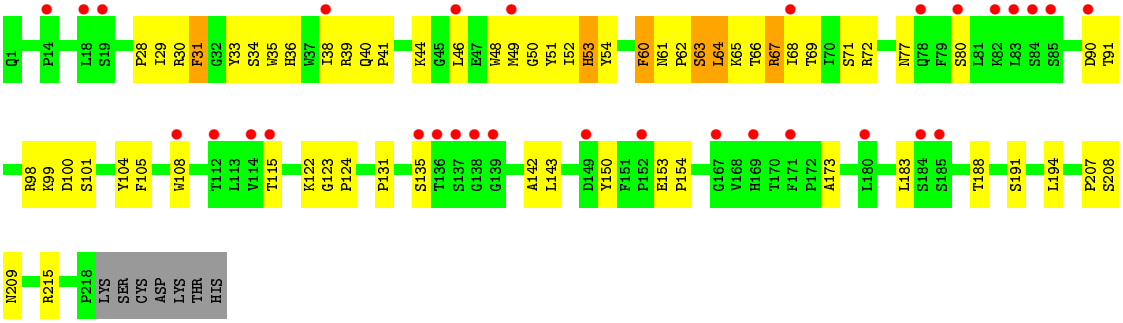
• Molecule 1: Fab C2E3 Heavy chain

Chain Q:



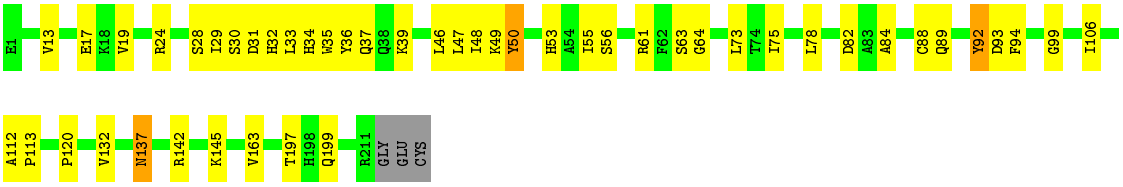
• Molecule 1: Fab C2E3 Heavy chain

Chain S:



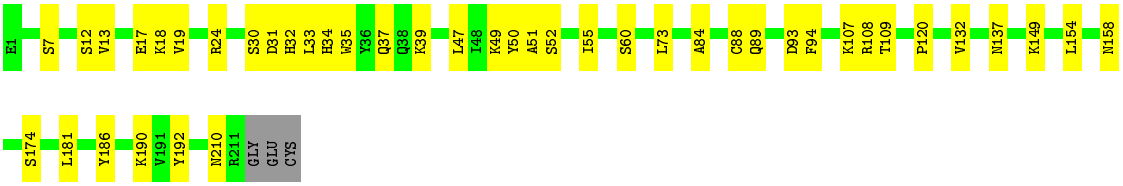
• Molecule 2: Fab C2E3 Light chain

Chain B:



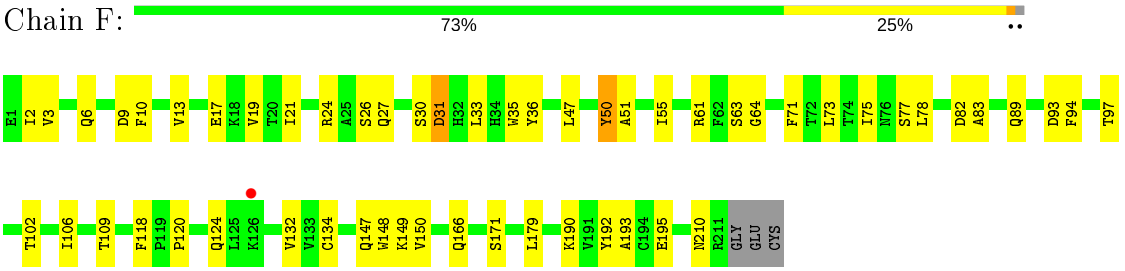
• Molecule 2: Fab C2E3 Light chain

Chain D:



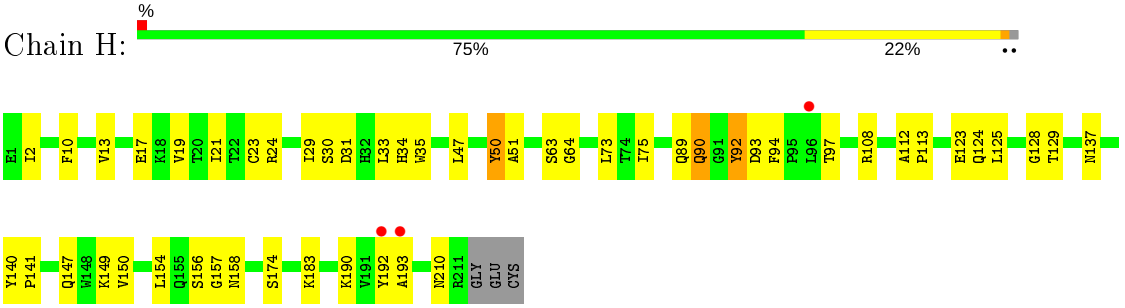
• Molecule 2: Fab C2E3 Light chain

Chain F:



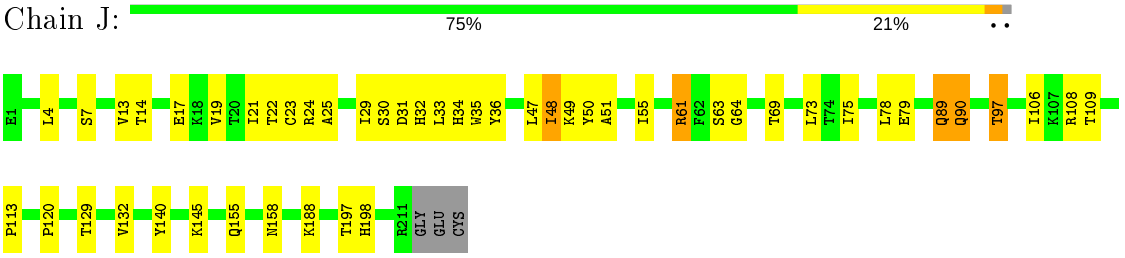
• Molecule 2: Fab C2E3 Light chain

Chain H:



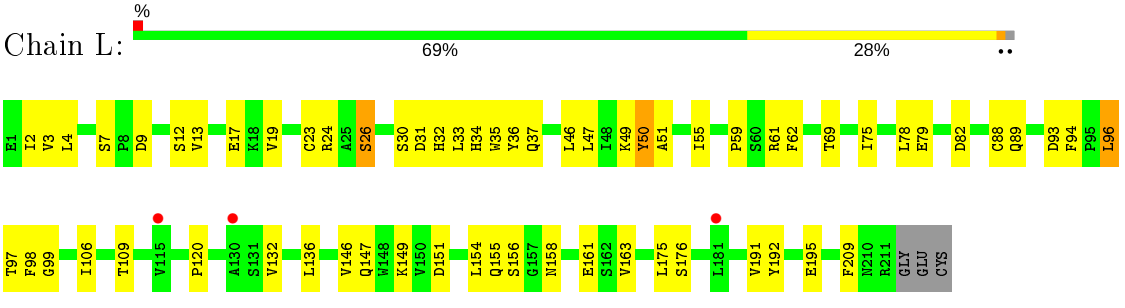
• Molecule 2: Fab C2E3 Light chain

Chain J:



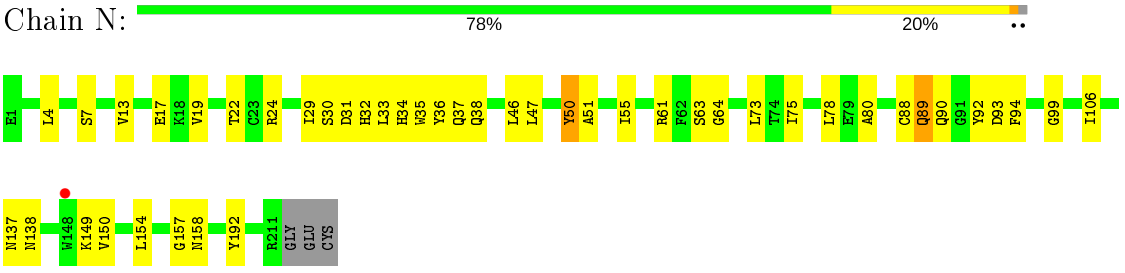
• Molecule 2: Fab C2E3 Light chain

Chain L:



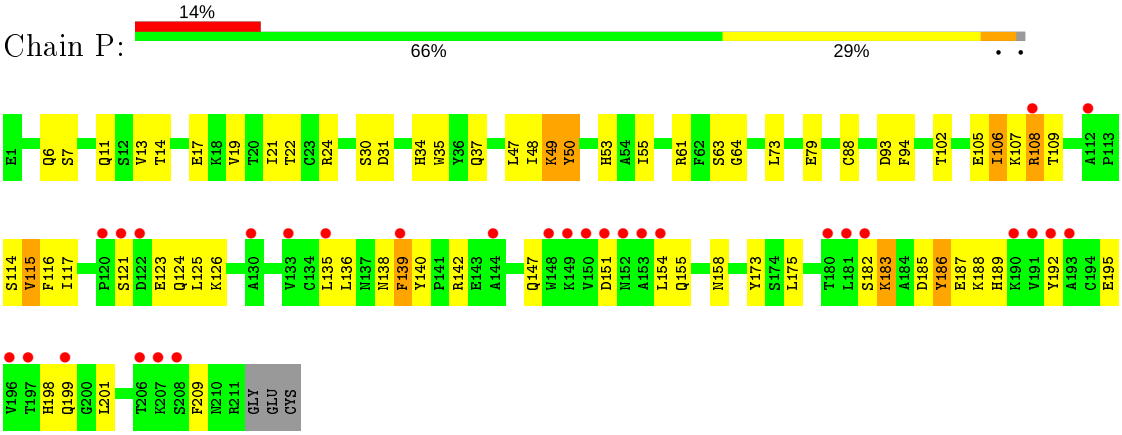
• Molecule 2: Fab C2E3 Light chain

Chain N:



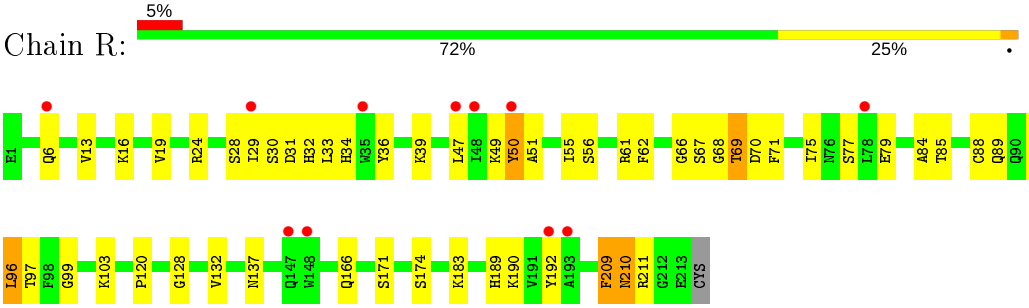
• Molecule 2: Fab C2E3 Light chain

Chain P:



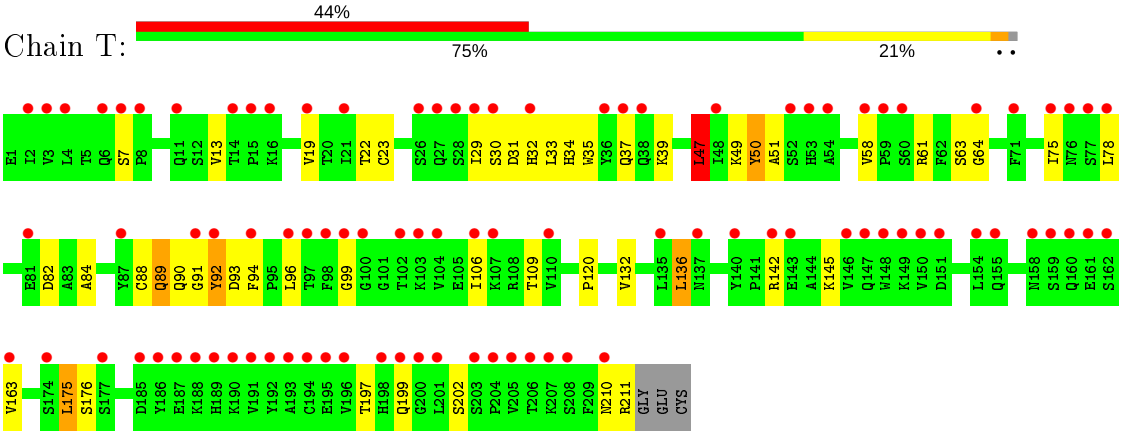
• Molecule 2: Fab C2E3 Light chain

Chain R:



• Molecule 2: Fab C2E3 Light chain

Chain T:



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 0.238 , 0.282	Depositor DCC
R_{free} test set	5006 reflections (4.75%)	wwPDB-VP
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 , 93.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	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
1:I:164:LEU:HD21	1:I:187:VAL:HG21	1.69	0.75
2:L:136:LEU:HD12	2:L:175:LEU:HB3	1.69	0.75
2:L:163:VAL:HG22	2:L:175:LEU:HG	1.69	0.74
1:C:51:TYR:HE1	1:C:59:ASP:HB3	1.53	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
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
1:Q:36:HIS:NE2	1:Q:99:LYS:HB2	2.03	0.73
2:T:37:GLN:HB2	2:T:47:LEU:HD21	1.70	0.73
1:G:33:TYR:O	1:G:35:TRP:NE1	2.22	0.73
2:P:6:GLN:HE21	2:P:102:THR:HG23	1.52	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:G:36:HIS:NE2	1:G:99:LYS:HB2	2.06	0.71
1:M:208:SER:O	1:S:215:ARG:NH1	2.24	0.71
1:S:41:PRO:HG2	1:S:44:LYS:HB2	1.73	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:H:30:SER:OG	2:H:31:ASP:N	2.25	0.70
2:L:30:SER:OG	2:L:31:ASP:N	2.24	0.70
1:K:36:HIS:HD2	1:K:48:TRP:HE1	1.39	0.70
1:O:33:TYR:H	1:O:33:TYR:HD1	1.39	0.70
2:P:151:ASP:OD2	2:P:189:HIS:ND1	2.25	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:40:GLN:HB2	1:S:46:LEU:HD23	1.75	0.68
1:S:36:HIS:NE2	1:S:99:LYS:HB2	2.09	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:O:22:CYS:HB3	1:O:79:PHE:HB2	1.77	0.66
1:Q:61:ASN:O	1:Q:65:LYS:HG3	1.95	0.66
2:P:155:GLN:OE1	2:P:158:ASN:ND2	2.29	0.66
1:E:40:GLN:HB2	1:E:46:LEU:HD13	1.78	0.66
1:K:48:TRP:HZ2	1:K:51:TYR:HD2	1.43	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
2:B:46:LEU:HG	2:B:55:ILE:HG13	1.77	0.65
1:E:32:GLY:H	1:E:54:TYR:HD2	1.44	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
1:O:8:GLY:HA3	1:O:20:LEU:HD23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:24:ARG:NH2	2:P:17:GLU:OE2	2.29	0.64
1:O:149:ASP:HA	1:O:180:LEU:HB3	1.79	0.64
2:L:93:ASP:OD1	2:L:94:PHE:N	2.30	0.64
1:M:29:ILE:HG22	1:M:35:TRP:CE2	2.32	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
1:G:48:TRP:HZ2	1:G:51:TYR:HD2	1.44	0.64
2:R:192:TYR:HB2	2:R:209:PHE:HE1	1.61	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
2:B:17:GLU:OE2	2:J:24:ARG:NH2	2.30	0.64
1:I:91:THR:HG23	1:I:115:THR:HA	1.79	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:G:61:ASN:OD1	1:G:63:SER:OG	2.14	0.62
1:M:33:TYR:O	1:M:35:TRP:NE1	2.31	0.62
2:F:61:ARG:NH2	2:F:82:ASP:OD1	2.27	0.62
1:O:33:TYR:N	1:O:33:TYR:CD1	2.67	0.62
1:I:51:TYR:HE1	1:I:59:ASP:HB3	1.64	0.62
1:K:36:HIS:HE1	1:K:99:LYS:HB2	1.61	0.62
1:A:98:ARG:HH21	1:A:106:PRO:HG3	1.65	0.62
1:S:29:ILE:HG13	1:S:77:ASN:OD1	2.00	0.62
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.81	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
1:A:91:THR:HG23	1:A:115:THR:HA	1.82	0.62
1:M:40:GLN:HB3	1:M:46:LEU:HD23	1.81	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
2:B:36:TYR:HE1	2:B:89:GLN:HG2	1.65	0.61
1:E:29:ILE:HG22	1:E:35:TRP:CE2	2.35	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
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.33	0.61
2:R:50:TYR:N	2:R:51:ALA:HA	2.15	0.61
1:S:33:TYR:O	1:S:35:TRP:NE1	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: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:106:ILE:H	2:P:106:ILE:HD12	1.66	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
1:M:124:PRO:HB3	1:M:150:TYR:HB3	1.85	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
2:R:30:SER:OG	2:R:31:ASP:N	2.35	0.59
2:B:24:ARG:NH2	2:J:17:GLU:OE2	2.35	0.59
1:M:215:ARG:NH2	1:S:209:ASN:H	1.98	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
1:I:149:ASP:HA	1:I:180:LEU:HB3	1.85	0.58
2:P:105:GLU:HG3	2:P:106:ILE:HD12	1.84	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
1:O:173:ALA:HA	1:O:183:LEU:HD13	1.85	0.58
2:P:11:GLN:O	2:P:105:GLU:N	2.31	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
1:K:11:LEU:HB2	1:K:152:PRO:HG3	1.86	0.58
2:R:36:TYR:OH	2:R:89:GLN:NE2	2.36	0.58
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:Q:61:ASN:OD1	1:Q:63:SER:OG	2.21	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
1:S:67:ARG:NH2	1:S:90:ASP:OD1	2.34	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:C:202:ASN:ND2	1:C:213:ASP:OD2	2.37	0.57
1:G:164:LEU:HD21	1:G:187:VAL:HG21	1.87	0.57
1:S:123:GLY:H	1:S:124:PRO:HD3	1.70	0.57
2:J:78:LEU:HD11	2:J:106:ILE:HG12	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
1:Q:91:THR:HG23	1:Q:115:THR:HA	1.87	0.57
2:T:34:HIS:HD2	2:T:89:GLN:HE21	1.52	0.57
2:J:50:TYR:N	2:J:51:ALA:HA	2.20	0.57
2:L:49:LYS:HG2	2:L:50:TYR:HD2	1.69	0.57
1:O:81:LEU:HD12	1:O:82:LYS:N	2.20	0.57
1:S:30:ARG:HA	1:S:54:TYR:HB2	1.87	0.56
1:O:53:HIS:CE1	1:O:54:TYR:CE2	2.94	0.56
1:E:48:TRP:HZ2	1:E:51:TYR:HD2	1.54	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
2:F:13:VAL:HB	2:F:78:LEU:HD22	1.86	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:19:VAL:HB	2:F:75:ILE:HB	1.88	0.56
2:T:136:LEU:HD11	2:T:175:LEU:HB3	1.86	0.56
1:A:36:HIS:HE2	1:A:99:LYS:HB2	1.69	0.56
2:J:33:LEU:HB3	2:J:51:ALA:HB2	1.86	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:C:148:LYS:NZ	1:C:176:GLN:OE1	2.34	0.55
1:E:98:ARG:HG2	1:E:100:ASP:H	1.71	0.55
2:T:30:SER:OG	2:T:31:ASP:N	2.39	0.55
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.40	0.55
2:J:4:LEU:HD21	2:J:90:GLN:HG3	1.87	0.55
2:N:19:VAL:HB	2:N:75:ILE:HB	1.89	0.55
2:P:6:GLN:NE2	2:P:102:THR:HG23	2.21	0.55
2:R:16:LYS:HA	2:R:77:SER:HB2	1.89	0.55
1:E:36:HIS:HE1	1:E:99:LYS:HB2	1.70	0.55
1:K:53:HIS:HD2	1:K:57:TYR:CE2	2.24	0.55
1:K:98:ARG:HH21	1:K:107:TYR:HE2	1.54	0.55
2:R:93:ASP:OD1	2:R:94:PHE:N	2.40	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
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:D:190:LYS:HE3	2:D:210:ASN:HB3	1.87	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
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:B:120:PRO:HD3	2:B:132:VAL:HG22	1.89	0.54
2:L:89:GLN:HB3	2:L:98:PHE:CD1	2.43	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:B:55:ILE:O	2:B:56:SER:HB3	2.08	0.53
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.88	0.53
2:N:4:LEU:HD21	2:N:90:GLN:HB3	1.90	0.53
1:Q:33:TYR:O	1:Q:35:TRP:NE1	2.41	0.53
2:H:19:VAL:HB	2:H:75:ILE:HB	1.90	0.53
2:T:136:LEU:HD11	2:T:175:LEU:HD22	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
1:I:33:TYR:HB2	1:I:98:ARG:HD2	1.90	0.53
2:P:14:THR:HG22	2:P:107:LYS:HE3	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:61:ASN:ND2	1:M:62:PRO:O	2.41	0.53
1:M:54:TYR:O	1:M:72:ARG:NH1	2.41	0.53
1:C:41:PRO:HB2	1:C:44:LYS:HB2	1.90	0.52
2:H:93:ASP:OD1	2:H:94:PHE:N	2.41	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
1:K:191:SER:HA	1:K:194:LEU:HD13	1.90	0.52
2:P:108:ARG:HE	2:P:108:ARG:HA	1.75	0.52
2:D:108:ARG:NH1	2:D:109:THR:O	2.43	0.52
2:L:32:HIS:ND1	2:L:50:TYR:HE1	2.08	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:F:149:LYS:HB2	2:F:193:ALA:HB3	1.91	0.51
2:L:175:LEU:HD23	2:L:176:SER:N	2.25	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
1:Q:205:HIS:CD2	1:Q:207:PRO:HD2	2.46	0.51
2:T:19:VAL:HB	2:T:75:ILE:HB	1.92	0.51
2:T:61:ARG:NH2	2:T:82:ASP:OD1	2.44	0.51
1:O:143:LEU:HB2	1:O:216:VAL:HG11	1.92	0.51
2:R:47:LEU:HD21	2:R:62:PHE:HD2	1.76	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:E:96:CYS:O	1:E:109:GLY:N	2.44	0.51
1:Q:62:PRO:HD3	2:R:95:PRO:HG2	1.92	0.51
1:C:18:LEU:N	1:C:83:LEU:O	2.38	0.50
2:P:116:PHE:O	2:P:135:LEU:N	2.36	0.50
2:B:78:LEU:HD11	2:B:106:ILE:HG12	1.93	0.50
2:L:155:GLN:OE1	2:L:158:ASN:ND2	2.35	0.50
1:S:65:LYS:O	1:S:68:ILE:HG22	2.11	0.50
1:A:143:LEU:H	1:A:143:LEU:HD12	1.76	0.50
2:D:93:ASP:OD1	2:D:94:PHE:N	2.44	0.50
2:F:93:ASP:OD1	2:F:94:PHE:N	2.44	0.50
1:M:173:ALA:HB2	1:M:183:LEU:HD23	1.92	0.50
1:A:32:GLY:O	1:A:54:TYR:HD2	1.94	0.50
2:D:137:ASN:O	2:D:174:SER:OG	2.17	0.50
1:E:100:ASP:OD1	1:E:101:SER:N	2.43	0.50
1:G:52:ILE:HG13	1:G:58:THR:HG22	1.92	0.50
1:K:104:TYR:HD1	2:L:46:LEU:HD11	1.76	0.50
1:Q:48:TRP:HZ2	1:Q:51:TYR:HD2	1.58	0.50
1:M:173:ALA:HA	1:M:183:LEU:HB3	1.94	0.50
2:T:33:LEU:HB3	2:T:51:ALA:HB2	1.93	0.50
2:T:90:GLN:NE2	2:T:96:LEU:HA	2.21	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: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
2:H:63:SER:OG	2:H:64:GLY:N	2.45	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
1:M:104:TYR:HB3	2:N:34:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2:VAL:HG22	1:O:27:TYR:HB2	1.94	0.49
1:O:33:TYR:HD2	1:O:100:ASP:HA	1.77	0.49
2:R:66:GLY:HA3	2:R:71:PHE:HD1	1.75	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
1:C:72:ARG:HA	1:C:79:PHE:HA	1.94	0.49
1:M:40:GLN:NE2	2:N:38:GLN:OE1	2.39	0.49
2:P:21:ILE:HB	2:P:73:LEU:HB3	1.93	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:S:28:PRO:HA	1:S:77:ASN:HD21	1.75	0.49
1:C:124:PRO:CB	1:C:150:TYR:HB3	2.36	0.49
2:F:78:LEU:HD21	2:F:106:ILE:HG13	1.94	0.49
1:O:164:LEU:HD11	1:O:189:VAL:HG21	1.95	0.49
1:O:127:PHE:CZ	2:P:124:GLN:HB3	2.48	0.49
1:Q:29:ILE:HG22	1:Q:35:TRP:CE2	2.47	0.49
2:R:19:VAL:HB	2:R:75:ILE:HB	1.94	0.49
2:T:145:LYS:HB3	2:T:197:THR:HB	1.95	0.49
1:A:104:TYR:HB3	2:B:34:HIS:CE1	2.47	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:C:30:ARG:HD2	1:M:180:LEU:HD21	1.93	0.49
1:K:168:VAL:HG12	1:K:187:VAL:HB	1.94	0.49
2:L:136:LEU:HD11	2:L:146:VAL:CG2	2.43	0.49
2:L:151:ASP:HA	2:L:191:VAL:HG23	1.94	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: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
1:I:11:LEU:HB3	1:I:152:PRO:HG3	1.95	0.48
2:R:128:GLY:HA2	2:R:183:LYS:HE2	1.94	0.48
1:Q:41:PRO:HB2	1:Q:44:LYS:HB2	1.94	0.48
2:R:47:LEU:HD21	2:R:62:PHE:CD2	2.47	0.48
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.48	0.48
2:D:24:ARG:NH2	2:F:17:GLU:OE2	2.41	0.48
2:F:61:ARG:HD2	2:F:77:SER:O	2.12	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:H:10:PHE:HB3	2:L:12:SER:HB3	1.95	0.48
2:N:47:LEU:O	2:N:55:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLU:HG2	1:A:154:PRO:HA	1.94	0.48
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:39:ARG:HD3	1:A:49:MET:HE3	1.96	0.48
1:O:129:LEU:HD22	1:O:144:GLY:H	1.79	0.48
2:P:49:LYS:HD3	2:P:50:TYR:CE1	2.49	0.48
1:Q:208:SER:OG	1:Q:209:ASN:N	2.46	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:E:127:PHE:CE1	2:F:124:GLN:HG2	2.48	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:G:96:CYS:O	1:G:109:GLY:N	2.47	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
2:B:48:ILE:HG22	2:B:49:LYS:O	2.13	0.47
1:E:41:PRO:HB2	1:E:44:LYS:HB2	1.96	0.47
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:O:18:LEU:HD22	1:O:19:SER:N	2.29	0.47
2:R:36:TYR:HE1	2:R:89:GLN:HG2	1.78	0.47
1:S:33:TYR:HB2	1:S:98:ARG:HG3	1.96	0.47
2:H:149:LYS:HB2	2:H:193:ALA:HB3	1.97	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:D:186:TYR:O	2:D:192:TYR:OH	2.31	0.47
1:E:27:TYR:CE2	1:E:32:GLY:HA3	2.37	0.47
2:N:35:TRP:CE2	2:N:73:LEU:HB2	2.50	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:R:96:LEU:HD23	2:R:97:THR:H	1.78	0.47
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.47
1:E:129:LEU:HG	1:E:130:ALA:N	2.27	0.47
2:H:21:ILE:HD12	2:H:73:LEU:HD23	1.97	0.47
1:K:124:PRO:CB	1:K:150:TYR:HB3	2.33	0.47
1:O:33:TYR:CD2	1:O:100:ASP:HA	2.49	0.47
2:P:63:SER:OG	2:P:64:GLY:N	2.47	0.47
1:S:36:HIS:CG	1:S:105:PHE:HE2	2.31	0.47
1:I:2:VAL:HG22	1:I:27:TYR:HB2	1.95	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:O:100:ASP:OD1	1:O:101:SER:N	2.46	0.47
2:T:7:SER:HG	2:T:22:THR:HG1	1.62	0.47
2:F:33:LEU:HG	2:F:71:PHE:CD2	2.50	0.47
1:O:18:LEU:O	1:O:83:LEU:N	2.40	0.47
2:J:47:LEU:HB3	2:J:48:ILE:HG12	1.96	0.47
1:S:52:ILE:HG12	1:S:53:HIS:O	2.14	0.47
1:A:135:SER:HA	1:A:191:SER:OG	2.14	0.47
1:A:173:ALA:HB2	1:A:183:LEU:HD23	1.96	0.47
2:B:145:LYS:HB3	2:B:197:THR:HB	1.96	0.47
2:F:2:ILE:O	2:F:97:THR:HG21	2.15	0.47
1:G:104:TYR:HB3	2:H:34:HIS:CE1	2.49	0.47
1:K:131:PRO:HG3	1:K:143:LEU:HB3	1.95	0.47
2:N:29:ILE:HA	2:N:92:TYR:CD2	2.50	0.47
2:P:186:TYR:CE2	2:P:187:GLU:HG2	2.49	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:T:199:GLN:OE1	2:T:199:GLN:N	2.45	0.47
1:E:142:ALA:HB2	1:E:188:THR:HG22	1.96	0.47
1:E:71:SER:O	1:E:80:SER:N	2.42	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
2:B:33:LEU:O	2:B:50:TYR:HA	2.15	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
1:C:35:TRP:CZ3	1:C:98:ARG:HD2	2.50	0.46
2:J:23:CYS:HB2	2:J:35:TRP:CH2	2.51	0.46
2:J:47:LEU:O	2:J:55:ILE:HG12	2.14	0.46
1:O:189:VAL:HG22	1:O:190:PRO:HD2	1.97	0.46
2:T:13:VAL:HG21	2:T:19:VAL:HG22	1.97	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: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
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.49	0.46
1:E:48:TRP:HZ2	1:E:51:TYR:CD2	2.33	0.46
2:H:128:GLY:HA2	2:H:183:LYS:HE2	1.96	0.46
2:J:61:ARG:NH2	2:J:79:GLU:HG3	2.31	0.46
2:L:13:VAL:HG21	2:L:19:VAL:HG22	1.96	0.46
1:M:32:GLY:O	1:M:54:TYR:CD2	2.67	0.46
2:P:182:SER:O	2:P:186:TYR:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:62:PRO:O	1:S:65:LYS:HB2	2.14	0.46
1:G:214:LYS:NZ	2:H:123:GLU:OE1	2.39	0.46
2:H:190:LYS:HE3	2:H:210:ASN:HB3	1.97	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:D:13:VAL:HG21	2:D:19:VAL:HG22	1.97	0.46
1:M:131:PRO:HG3	1:M:143:LEU:HB3	1.97	0.46
2:P:136:LEU:N	2:P:175:LEU:O	2.35	0.46
1:C:88:ALA:O	1:C:91:THR:HG22	2.16	0.46
1:Q:72:ARG:HA	1:Q:79:PHE:HA	1.97	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: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:P:49:LYS:HG3	2:P:55:ILE:HD11	1.98	0.46
1:C:102:GLY:HA3	2:D:50:TYR:OH	2.15	0.46
1:C:48:TRP:CE3	1:C:61:ASN:HB2	2.51	0.46
2:J:34:HIS:CE1	2:J:49:LYS:NZ	2.83	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:S:61:ASN:OD1	1:S:63:SER:N	2.48	0.46
1:I:148:LYS:NZ	1:I:176:GLN:OE1	2.37	0.45
1:K:151:PHE:HA	1:K:152:PRO:HA	1.77	0.45
1:K:142:ALA:HB2	1:K:188:THR:HG22	1.99	0.45
1:M:158:SER:O	1:M:159:TRP:HD1	1.99	0.45
1:O:179:GLY:O	1:O:180:LEU:HD13	2.15	0.45
1:O:48:TRP:HZ2	1:O:51:TYR:CD2	2.29	0.45
1:Q:29:ILE:HD12	1:Q:30:ARG:N	2.31	0.45
1:S:135:SER:HA	1:S:191:SER:OG	2.16	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
2:D:39:LYS:HG2	2:D:84:ALA:HB2	1.98	0.45
1:G:173:ALA:HB2	1:G:183:LEU:HD23	1.97	0.45
1:G:71:SER:O	1:G:80:SER:N	2.45	0.45
1:K:30:ARG:O	1:K:54:TYR:HB2	2.16	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:Q:27:TYR:HE1	1:Q:31:PHE:O	1.99	0.45
2:B:199:GLN:OE1	2:B:199:GLN:N	2.44	0.45
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:157:GLY:HA3	2:P:154:LEU:HD11	1.97	0.45
1:Q:29:ILE:HG13	1:Q:29:ILE:H	1.57	0.45
2:D:158:ASN:OD1	2:D:158:ASN:N	2.49	0.45
1:E:33:TYR:CD1	1:E:33:TYR:N	2.84	0.45
1:K:36:HIS:HD2	1:K:48:TRP:NE1	2.10	0.45
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.99	0.45
2:B:35:TRP:CG	2:B:73:LEU:HD12	2.52	0.45
2:D:149:LYS:HG2	2:D:154:LEU:HD23	1.99	0.45
2:D:35:TRP:CG	2:D:73:LEU:HD12	2.51	0.45
1:K:103:ASN:HB3	2:L:96:LEU:CD2	2.47	0.45
1:O:123:GLY:HA2	1:O:124:PRO:HD3	1.69	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
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
1:Q:18:LEU:N	1:Q:83:LEU:O	2.38	0.45
2:T:88:CYS:O	2:T:99:GLY:N	2.48	0.45
2:T:90:GLN:N	2:T:90:GLN:OE1	2.45	0.45
2:J:49:LYS:HG2	2:J:50:TYR:CD2	2.52	0.45
1:K:28:PRO:HG2	1:K:31:PHE:CD2	2.52	0.45
2:N:93:ASP:OD1	2:N:94:PHE:N	2.50	0.45
1:O:171:PHE:HA	1:O:172:PRO:HD3	1.83	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:CG	2.52	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:A:113:LEU:HD12	1:A:114:VAL:H	1.82	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:S:31:PHE:N	1:S:31:PHE:CD1	2.83	0.45
1:A:168:VAL:HG22	1:A:187:VAL:HB	1.98	0.44
1:A:53:HIS:HB2	1:A:57:TYR:HB3	1.99	0.44
1:E:143:LEU:O	1:E:187:VAL:N	2.36	0.44
2:D:12:SER:HB3	2:F:10:PHE:HB3	1.99	0.44
1:G:29:ILE:HG13	1:G:77:ASN:OD1	2.18	0.44
1:O:200:ILE:HG22	1:O:215:ARG:HA	1.99	0.44
1:E:34:SER:HB2	1:E:36:HIS:CE1	2.45	0.44
2:F:147:GLN:HB3	2:F:195:GLU:HB3	1.99	0.44
1:K:104:TYR:O	1:K:106:PRO:HD3	2.17	0.44
1:A:27:TYR:OH	1:A:32:GLY:HA3	2.17	0.44
2:D:158:ASN:HD22	2:D:181:LEU:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:61:ARG:HH22	2:J:79:GLU:HG3	1.82	0.44
1:K:33:TYR:CD2	1:K:100:ASP:HA	2.52	0.44
2:R:49:LYS:C	2:R:51:ALA:HA	2.37	0.44
2:H:112:ALA:HA	2:H:113:PRO:HD3	1.83	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
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:S:39:ARG:HD3	1:S:49:MET:HE3	2.00	0.44
1:I:36:HIS:CD2	1:I:51:TYR:HB2	2.52	0.44
2:J:188:LYS:HE2	2:J:188:LYS:HB3	1.83	0.44
2:J:30:SER:O	2:J:32:HIS:N	2.44	0.44
1:O:35:TRP:CG	1:O:79:PHE:CE1	3.06	0.44
1:O:52:ILE:HA	1:O:58:THR:HG22	2.00	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
1:S:131:PRO:HB3	1:S:143:LEU:HB3	2.00	0.44
1:S:71:SER:O	1:S:80:SER:N	2.36	0.44
2:B:46:LEU:O	2:B:55:ILE:HG21	2.18	0.44
2:F:166:GLN:HE21	2:F:171:SER:HB3	1.83	0.44
2:H:150:VAL:HG13	2:H:192:TYR:CE1	2.52	0.44
2:T:49:LYS:C	2:T:51:ALA:HA	2.38	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:O:104:TYR:HB3	2:P:34:HIS:CE1	2.53	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
2:R:33:LEU:HD13	2:R:34:HIS:N	2.33	0.44
1:A:98:ARG:NH2	1:A:100:ASP:OD2	2.51	0.43
1:I:29:ILE:HD11	1:I:77:ASN:C	2.39	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:E:164:LEU:HD11	1:E:187:VAL:HG21	1.99	0.43
1:E:204:ASN:HB2	1:E:211:LYS:HE2	1.99	0.43
1:E:54:TYR:HD1	1:E:55:SER:N	2.16	0.43
2:H:63:SER:O	2:H:73:LEU:HD12	2.18	0.43
2:P:107:LYS:HD3	2:P:109:THR:CB	2.48	0.43
1:Q:173:ALA:HB2	1:Q:183:LEU:HD23	2.00	0.43
2:T:78:LEU:HD11	2:T:106:ILE:HG12	2.01	0.43
1:G:29:ILE:HG22	1:G:35:TRP:NE1	2.32	0.43
2:H:33:LEU:HD22	2:H:89:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ARG:HA	1:K:79:PHE:HA	2.00	0.43
2:P:7:SER:OG	2:P:22:THR:OG1	2.21	0.43
1:O:192:SER:HA	1:Q:66:THR:HA	1.99	0.43
1:I:18:LEU:N	1:I:83:LEU:O	2.42	0.43
1:K:54:TYR:CD1	1:K:55:SER:N	2.87	0.43
2:L:33:LEU:HG	2:L:34:HIS:N	2.33	0.43
1:O:27:TYR:HA	1:O:28:PRO:HD3	1.74	0.43
2:P:21:ILE:HG23	2:P:102:THR:HG21	2.00	0.43
2:R:85:THR:HG22	2:R:103:LYS:HG3	2.00	0.43
2:R:67:SER:OG	2:R:68:GLY:N	2.51	0.43
1:C:33:TYR:N	1:C:33:TYR:CD2	2.85	0.43
1:E:10:GLY:HA3	1:E:207:PRO:HG3	2.01	0.43
2:J:129:THR:HG23	1:Q:76:LYS:HE2	1.99	0.43
2:N:33:LEU:HD12	2:N:89:GLN:O	2.18	0.43
2:T:142:ARG:HE	2:T:163:VAL:HG11	1.83	0.43
2:B:112:ALA:HA	2:B:113:PRO:HD3	1.86	0.43
2:B:142:ARG:HE	2:B:163:VAL:HG11	1.84	0.43
1:C:53:HIS:HB2	1:C:57:TYR:CB	2.49	0.43
1:I:33:TYR:N	1:I:33:TYR:CD1	2.87	0.43
2:J:145:LYS:HB3	2:J:197:THR:OG1	2.19	0.43
1:M:98:ARG:HH21	1:M:107:TYR:HE2	1.64	0.43
1:O:129:LEU:HB3	1:O:144:GLY:O	2.18	0.43
2:B:39:LYS:HG2	2:B:84:ALA:HB2	2.01	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:D:7:SER:HB2	2:F:13:VAL:HG13	2.00	0.43
2:F:21:ILE:HB	2:F:73:LEU:HB3	2.00	0.43
2:F:36:TYR:HE1	2:F:89:GLN:CG	2.32	0.43
2:H:158:ASN:N	2:H:158:ASN:OD1	2.51	0.43
1:M:36:HIS:HE2	1:M:99:LYS:HB2	1.77	0.43
2:P:136:LEU:HB3	2:P:139:PHE:CE1	2.53	0.43
1:A:205:HIS:CD2	1:A:207:PRO:HD2	2.54	0.43
2:J:155:GLN:OE1	2:J:158:ASN:ND2	2.41	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
1:A:8:GLY:HA3	1:A:20:LEU:HD23	2.01	0.43
1:C:37:TRP:HB3	1:C:49:MET:HE3	2.00	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:35:TRP:CD2	2:B:73:LEU:HD12	2.54	0.42
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
1:C:122:LYS:HD2	1:C:149:ASP:O	2.18	0.42
1:K:60:PHE:HE1	1:K:70:ILE:HG13	1.84	0.42
2:L:192:TYR:HB2	2:L:209:PHE:CE1	2.55	0.42
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.55	0.42
2:L:2:ILE:O	2:L:97:THR:HG21	2.19	0.42
2:B:13:VAL:HG21	2:B:19:VAL:HG22	2.01	0.42
1:O:151:PHE:HA	1:O:152:PRO:HA	1.82	0.42
1:Q:67:ARG:HH22	1:Q:86:VAL:HA	1.85	0.42
2:R:29:ILE:HB	2:R:71:PHE:HE2	1.85	0.42
1:A:151:PHE:HA	1:A:152:PRO:HA	1.83	0.41
2:D:18:LYS:HB3	2:D:18:LYS:HE2	1.81	0.41
1:E:60:PHE:O	1:E:65:LYS:NZ	2.53	0.41
2:H:89:GLN:HG2	2:H:90:GLN:N	2.34	0.41
2:J:108:ARG:HG2	2:J:140:TYR:CD2	2.55	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:L:61:ARG:NH1	2:L:79:GLU:HB2	2.35	0.41
2:N:17:GLU:OE2	2:P:24:ARG:NH2	2.28	0.41
2:N:47:LEU:HD23	2:N:47:LEU:HA	1.93	0.41
1:Q:62:PRO:HD3	2:R:95:PRO:CG	2.50	0.41
2:R:6:GLN:HE21	2:R:99:GLY:HA3	1.86	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:R:29:ILE:O	2:R:29:ILE:HG22	2.20	0.41
2:T:175:LEU:HD23	2:T:176:SER:N	2.35	0.41
1:C:123:GLY:HA2	1:C:124:PRO:HD3	1.84	0.41
1:G:32:GLY:O	1:G:54:TYR:CD2	2.73	0.41
2:H:124:GLN:HG2	2:H:129:THR:O	2.20	0.41
2:H:140:TYR:CG	2:H:141:PRO:HA	2.55	0.41
1:K:100:ASP:OD1	1:K:101:SER:N	2.50	0.41
1:K:106:PRO:HG2	1:K:107:TYR:CD2	2.55	0.41
1:A:122:LYS:O	1:A:205:HIS:HE1	2.04	0.41
2:F:134:CYS:HB2	2:F:148:TRP:CH2	2.56	0.41
1:I:100:ASP:OD1	1:I:101:SER:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:LYS:HB3	1:K:137:SER:HB2	2.02	0.41
2:H:157:GLY:HA3	2:L:154:LEU:HD13	2.03	0.41
1:O:104:TYR:O	1:O:106:PRO:HD3	2.21	0.41
1:Q:104:TYR:HB3	2:R:34:HIS:NE2	2.35	0.41
2:H:47:LEU:HA	2:H:47:LEU:HD23	1.94	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
1:C:173:ALA:HA	1:C:183:LEU:HB3	2.02	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:51:TYR:CE2	2:F:94:PHE:HE2	2.39	0.41
1:G:104:TYR:O	1:G:106:PRO:HD3	2.21	0.41
1:K:104:TYR:CZ	2:L:49:LYS:HE2	2.56	0.41
1:O:176:GLN:HG2	1:O:179:GLY:H	1.86	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:F:134:CYS:HB2	2:F:148:TRP:CZ2	2.54	0.41
2:F:33:LEU:HG	2:F:71:PHE:CG	2.56	0.41
1:G:65:LYS:HE3	1:G:65:LYS:HB2	1.86	0.41
2:J:34:HIS:ND1	2:J:49:LYS:HG3	2.36	0.41
2:L:49:LYS:HZ2	2:L:50:TYR:HE2	1.67	0.41
1:M:48:TRP:CE3	1:M:61:ASN:HB2	2.56	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:D:47:LEU:O	2:D:55:ILE:HG12	2.21	0.41
1:G:212:VAL:HA	1:Q:211:LYS:O	2.21	0.41
1:I:168:VAL:HG12	1:I:187:VAL:HB	2.02	0.41
1:K:48:TRP:CZ2	1:K:50:GLY:HA2	2.56	0.41
2:N:158:ASN:OD1	2:N:158:ASN:N	2.54	0.41
2:N:7:SER:HG	2:N:22:THR:HG1	1.62	0.41
1:Q:217:GLU:HA	1:Q:218:PRO:HD3	1.92	0.41
1:S:34:SER:HB2	1:S:53:HIS:HA	2.02	0.41
2:T:29:ILE:HG22	2:T:92:TYR:HD2	1.85	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
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
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:I:53:HIS:CB	1:I:57:TYR:HB3	2.51	0.40
1:O:35:TRP:CG	1:O:79:PHE:HE1	2.39	0.40
1:S:29:ILE:HG13	1:S:29:ILE:H	1.75	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:L:4:LEU:HD12	2:L:23:CYS:SG	2.62	0.40
2:N:149:LYS:HG2	2:N:154:LEU:HD23	2.04	0.40
2:N:89:GLN:O	2:N:89:GLN:HG3	2.21	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
1:Q:63:SER:C	1:Q:64:LEU:HG	2.42	0.40
1:A:18:LEU:N	1:A:83:LEU:O	2.41	0.40
1:C:104:TYR:HB3	2:D:34:HIS:CE1	2.56	0.40
2:J:33:LEU:HD22	2:J:34:HIS:H	1.85	0.40
2:N:37:GLN:HB2	2:N:47:LEU:HD11	2.02	0.40
1:O:64:LEU:H	1:O:64:LEU:HG	1.63	0.40
2:P:136:LEU:HD22	2:P:139:PHE:HE1	1.86	0.40
1:S:191:SER:HA	1:S:194:LEU:HD13	2.03	0.40
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.88	0.40
1:E:33:TYR:HB2	1:E:98:ARG:HD2	2.04	0.40
2:H:149:LYS:HG2	2:H:154:LEU:HD23	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:M:31:PHE:N	1:M:31:PHE:CD1	2.89	0.40
2:N:13:VAL:HG13	2:P:7:SER:HB2	2.03	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:R:39:LYS:HG2	2:R:84:ALA:HB2	2.04	0.40
2:T:39:LYS:HG2	2:T:84:ALA:HB2	2.03	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%)	29	66
1	C	216/225 (96%)	206 (95%)	10 (5%)	0	100	100
1	E	216/225 (96%)	209 (97%)	6 (3%)	1 (0%)	29	66
1	G	216/225 (96%)	210 (97%)	5 (2%)	1 (0%)	29	66
1	I	216/225 (96%)	207 (96%)	9 (4%)	0	100	100
1	K	216/225 (96%)	209 (97%)	6 (3%)	1 (0%)	29	66
1	M	216/225 (96%)	210 (97%)	6 (3%)	0	100	100
1	O	216/225 (96%)	207 (96%)	8 (4%)	1 (0%)	29	66
1	Q	216/225 (96%)	207 (96%)	8 (4%)	1 (0%)	29	66
1	S	216/225 (96%)	206 (95%)	9 (4%)	1 (0%)	29	66
2	B	209/214 (98%)	201 (96%)	7 (3%)	1 (0%)	29	66
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%)	47	80

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%)	25	58
1	C	189/196 (96%)	179 (95%)	10 (5%)	22	54
1	E	189/196 (96%)	181 (96%)	8 (4%)	30	61
1	G	189/196 (96%)	184 (97%)	5 (3%)	46	74
1	I	189/196 (96%)	181 (96%)	8 (4%)	30	61
1	K	189/196 (96%)	181 (96%)	8 (4%)	30	61
1	M	189/196 (96%)	185 (98%)	4 (2%)	53	78
1	O	189/196 (96%)	173 (92%)	16 (8%)	10	38
1	Q	189/196 (96%)	185 (98%)	4 (2%)	53	78
1	S	189/196 (96%)	181 (96%)	8 (4%)	30	61
2	B	187/189 (99%)	181 (97%)	6 (3%)	39	69
2	D	187/189 (99%)	184 (98%)	3 (2%)	62	83
2	F	187/189 (99%)	184 (98%)	3 (2%)	62	83
2	H	187/189 (99%)	182 (97%)	5 (3%)	44	73
2	J	187/189 (99%)	180 (96%)	7 (4%)	34	64
2	L	187/189 (99%)	183 (98%)	4 (2%)	53	78
2	N	187/189 (99%)	183 (98%)	4 (2%)	53	78
2	P	187/189 (99%)	176 (94%)	11 (6%)	19	52
2	R	188/189 (100%)	182 (97%)	6 (3%)	39	69
2	T	187/189 (99%)	181 (97%)	6 (3%)	39	69
All	All	3761/3850 (98%)	3626 (96%)	135 (4%)	35	66

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%) 84 81	78, 111, 160, 222	0
1	C	218/225 (96%)	0.14	7 (3%) 47 46	91, 122, 177, 248	0
1	E	218/225 (96%)	0.46	15 (6%) 16 19	102, 159, 254, 334	0
1	G	218/225 (96%)	0.18	2 (0%) 84 81	84, 110, 166, 227	0
1	I	218/225 (96%)	0.32	9 (4%) 37 36	105, 141, 197, 248	0
1	K	218/225 (96%)	0.25	6 (2%) 53 51	111, 146, 197, 255	0
1	M	218/225 (96%)	0.19	7 (3%) 47 46	86, 120, 200, 273	0
1	O	218/225 (96%)	1.04	46 (21%) 1 1	120, 192, 301, 337	0
1	Q	218/225 (96%)	0.25	7 (3%) 47 46	102, 138, 186, 228	0
1	S	218/225 (96%)	0.88	31 (14%) 2 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%) 75 72	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%) 75 72	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%) 2 4	109, 191, 319, 344	0
2	R	213/214 (99%)	0.47	11 (5%) 27 27	109, 152, 202, 223	0
2	T	211/214 (98%)	1.99	94 (44%) 0 0	186, 255, 312, 338	0
All	All	4292/4390 (97%)	0.37	275 (6%) 19 20	78, 139, 262, 344	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	181	LEU	16.8
1	S	136	THR	13.5
1	O	131	PRO	13.0
2	P	149	LYS	10.2
1	E	136	THR	9.8
1	O	189	VAL	8.6
2	P	191	VAL	8.6
2	P	206	THR	8.2
1	O	165	THR	7.8
2	T	104	VAL	7.6
2	P	151	ASP	7.2
1	E	137	SER	7.1
2	T	2	ILE	6.8
1	O	188	THR	6.8
1	E	135	SER	6.7
1	S	83	LEU	6.7
2	T	29	ILE	6.5
2	T	194	CYS	6.4
2	T	11	GLN	6.3
2	P	122	ASP	6.0
1	O	193	SER	6.0
1	Q	136	THR	6.0
2	T	148	TRP	6.0
2	P	180	THR	5.8
1	C	135	SER	5.7
1	O	190	PRO	5.6
2	T	159	SER	5.5
1	O	164	LEU	5.5
2	P	153	ALA	5.5
2	T	28	SER	5.4
2	P	121	SER	5.4
1	Q	135	SER	5.3
2	T	207	LYS	5.3
1	O	145	CYS	5.3
1	Q	137	SER	5.3
2	T	191	VAL	5.3
1	O	162	GLY	5.2
2	T	149	LYS	5.2
2	T	78	LEU	5.1
2	T	190	LYS	5.0
2	P	208	SER	5.0
2	T	75	ILE	5.0
1	I	136	THR	5.0

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Mol	Chain	Res	Type	RSRZ
2	T	200	GLY	5.0
1	O	199	TYR	5.0
2	P	207	LYS	5.0
2	P	154	LEU	4.9
2	P	190	LYS	4.8
1	O	163	ALA	4.8
2	T	77	SER	4.8
1	I	135	SER	4.8
1	O	126	VAL	4.7
1	S	137	SER	4.7
1	O	159	TRP	4.6
1	S	82	LYS	4.6
2	T	19	VAL	4.6
1	M	136	THR	4.5
2	T	193	ALA	4.5
2	T	186	TYR	4.5
2	T	30	SER	4.4
2	T	147	GLN	4.4
2	T	96	LEU	4.4
1	S	138	GLY	4.4
1	A	135	SER	4.4
1	S	135	SER	4.3
1	O	132	SER	4.3
2	T	15	PRO	4.3
1	O	213	ASP	4.3
2	T	59	PRO	4.2
2	P	130	ALA	4.2
1	O	161	SER	4.2
2	T	204	PRO	4.2
1	O	194	LEU	4.0
2	T	8	PRO	4.0
1	A	136	THR	3.9
1	E	194	LEU	3.9
1	O	218	PRO	3.9
1	O	166	SER	3.8
1	C	137	SER	3.8
1	O	200	ILE	3.8
2	T	137	ASN	3.7
1	E	128	PRO	3.7
2	T	92	TYR	3.7
1	O	138	GLY	3.7
2	R	147	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	138	GLY	3.7
2	T	208	SER	3.7
1	C	136	THR	3.6
2	T	189	HIS	3.6
1	M	135	SER	3.6
2	L	181	LEU	3.6
2	P	196	VAL	3.6
2	T	205	VAL	3.6
2	T	177	SER	3.6
1	O	150	TYR	3.6
2	T	107	LYS	3.6
2	T	98	PHE	3.5
2	T	48	ILE	3.5
2	T	155	GLN	3.5
1	E	199	TYR	3.5
1	K	135	SER	3.5
1	O	130	ALA	3.5
2	T	54	ALA	3.5
1	S	114	VAL	3.5
2	P	197	THR	3.4
1	S	185	SER	3.4
2	P	139	PHE	3.4
2	T	64	GLY	3.4
1	S	46	LEU	3.4
1	O	136	THR	3.4
2	T	196	VAL	3.3
2	F	126	LYS	3.3
1	O	191	SER	3.2
2	R	148	TRP	3.2
2	T	97	THR	3.2
1	O	143	LEU	3.2
2	P	144	ALA	3.2
2	T	106	ILE	3.2
2	T	87	TYR	3.2
2	P	182	SER	3.1
1	O	196	THR	3.1
2	T	150	VAL	3.1
1	K	199	TYR	3.1
2	T	38	GLN	3.1
2	R	35	TRP	3.1
2	P	135	LEU	3.1
1	S	38	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	S	171	PHE	3.1
2	R	6	GLN	3.0
2	T	103	LYS	3.0
1	I	199	TYR	3.0
1	S	18	LEU	3.0
2	T	110	VAL	3.0
1	O	147	VAL	3.0
2	T	151	ASP	3.0
1	O	160	ASN	3.0
1	O	181	TYR	3.0
2	T	7	SER	2.9
2	T	158	ASN	2.9
2	T	102	THR	2.9
2	R	29	ILE	2.9
1	E	190	PRO	2.9
2	T	203	SER	2.9
1	E	115	THR	2.9
1	S	49	MET	2.9
1	G	135	SER	2.9
1	I	138	GLY	2.9
2	T	188	LYS	2.9
1	M	141	ALA	2.9
1	I	145	CYS	2.8
1	K	136	THR	2.8
2	T	58	VAL	2.8
2	T	198	HIS	2.8
1	E	130	ALA	2.8
2	T	135	LEU	2.8
2	T	210	ASN	2.8
1	S	80	SER	2.8
1	I	130	ALA	2.8
1	O	216	VAL	2.8
1	O	137	SER	2.8
2	T	162	SER	2.8
1	O	185	SER	2.8
2	T	71	PHE	2.7
1	K	216	VAL	2.7
2	T	91	GLY	2.7
2	T	185	ASP	2.7
2	T	16	LYS	2.7
2	T	36	TYR	2.7
1	G	136	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	T	6	GLN	2.7
2	P	150	VAL	2.6
1	Q	138	GLY	2.6
2	P	199	GLN	2.6
1	S	108	TRP	2.6
2	T	94	PHE	2.6
1	O	184	SER	2.6
1	S	85	SER	2.6
2	P	120	PRO	2.6
1	S	149	ASP	2.6
1	S	180	LEU	2.6
2	L	115	VAL	2.6
1	Q	83	LEU	2.6
1	S	112	THR	2.6
2	T	27	GLN	2.6
1	Q	105	PHE	2.6
2	H	193	ALA	2.6
2	T	206	THR	2.6
2	R	78	LEU	2.6
2	T	37	GLN	2.6
2	T	99	GLY	2.5
2	T	154	LEU	2.5
2	P	133	VAL	2.5
1	S	184	SER	2.5
1	O	144	GLY	2.5
2	P	108	ARG	2.5
2	R	192	TYR	2.5
1	E	150	TYR	2.5
1	C	138	GLY	2.5
2	P	192	TYR	2.5
2	T	26	SER	2.5
1	I	143	LEU	2.5
2	R	47	LEU	2.5
2	T	174	SER	2.5
2	T	142	ARG	2.5
2	T	76	ASN	2.4
1	S	169	HIS	2.4
2	T	4	LEU	2.4
1	S	19	SER	2.4
2	T	192	TYR	2.4
1	O	128	PRO	2.4
1	M	199	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	78	GLN	2.4
2	T	60	SER	2.4
2	T	195	GLU	2.4
2	T	201	LEU	2.4
1	O	152	PRO	2.4
2	L	130	ALA	2.4
1	O	135	SER	2.3
1	I	137	SER	2.3
1	S	84	SER	2.3
1	K	159	TRP	2.3
2	H	192	TYR	2.3
1	O	187	VAL	2.3
2	T	163	VAL	2.3
1	O	133	SER	2.3
2	T	187	GLU	2.3
1	S	152	PRO	2.3
2	T	199	GLN	2.3
1	S	167	GLY	2.3
2	T	21	ILE	2.3
2	T	161	GLU	2.2
1	M	143	LEU	2.2
2	T	3	VAL	2.2
2	T	53	HIS	2.2
2	H	96	LEU	2.2
1	O	60	PHE	2.2
1	O	198	THR	2.2
2	T	81	GLU	2.2
2	P	148	TRP	2.2
1	C	132	SER	2.2
1	O	158	SER	2.2
2	T	100	GLY	2.2
2	R	193	ALA	2.2
1	Q	47	GLU	2.2
1	O	203	VAL	2.2
2	T	140	TYR	2.2
2	T	160	GLN	2.2
1	C	143	LEU	2.2
1	S	68	ILE	2.2
2	P	112	ALA	2.1
2	P	152	ASN	2.1
1	E	196	THR	2.1
2	T	52	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	148	TRP	2.1
1	O	212	VAL	2.1
2	T	143	GLU	2.1
1	M	132	SER	2.1
1	C	194	LEU	2.1
1	K	184	SER	2.1
2	P	193	ALA	2.1
1	S	115	THR	2.1
1	S	139	GLY	2.1
1	O	192	SER	2.1
1	I	194	LEU	2.1
1	E	134	LYS	2.1
2	T	32	HIS	2.1
1	S	90	ASP	2.0
2	T	14	THR	2.0
1	E	12	VAL	2.0
1	M	142	ALA	2.0
1	S	14	PRO	2.0
2	R	48	ILE	2.0
1	E	70	ILE	2.0
2	R	50	TYR	2.0
2	T	146	VAL	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.