Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 08:15 PM EDT

PDB ID	:	4R7D
Title	:	Fab Hu 15C1
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	:	2014-08-27
Resolution	:	2.75 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

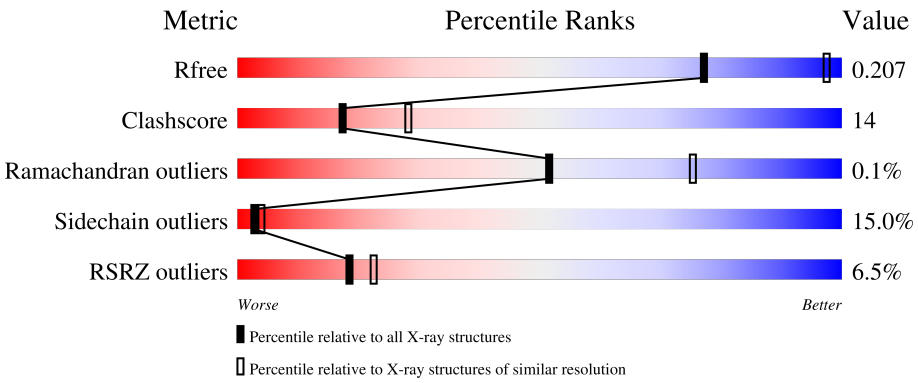
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	225	2%, 65%, 29%, • •
1	C	225	6%, 64%, 25%, •, 7%
1	E	225	8%, 59%, 29%, •, 7%
1	G	225	4%, 58%, 24%, •, 16%
1	I	225	4%, 65%, 27%, • •

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Mol	Chain	Length	Quality of chain
1	K	225	4% 61% 24% 11%
1	M	225	7% 59% 26% 11%
1	O	225	6% 60% 27% 6% 7%
2	B	214	% 57% 37% 5%
2	D	214	17% 65% 26% 7%
2	F	214	9% 61% 31% 7%
2	H	214	6% 57% 35% 7%
2	J	214	2% 61% 32% 7%
2	L	214	6% 58% 35% 5%
2	N	214	8% 59% 33% 7%
2	P	214	8% 59% 34% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26033 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 Hu 15C1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1641	1042	272	322	5	0	0	0
1	C	210	1593	1016	263	309	5	0	0	0
1	E	209	1584	1011	261	307	5	0	0	0
1	G	190	1445	927	236	277	5	0	0	0
1	I	218	1641	1042	272	322	5	0	0	0
1	K	201	1533	980	253	295	5	0	0	0
1	M	201	1533	980	253	295	5	0	0	0
1	O	209	1584	1011	261	307	5	0	0	0

- Molecule 2 is a protein called Fab Hu 15C1 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	211	1631	1023	275	329	4	0	0	0
2	D	211	1626	1020	275	327	4	0	0	0
2	F	211	1626	1020	275	327	4	0	0	0
2	H	212	1635	1025	276	330	4	0	0	0
2	J	212	1635	1025	276	330	4	0	0	0
2	L	211	1631	1023	275	329	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	211	1626	1020	275	327	4	0	0	0
			Total	C	N	O	S			
2	P	211	1626	1020	275	327	4	0	0	0

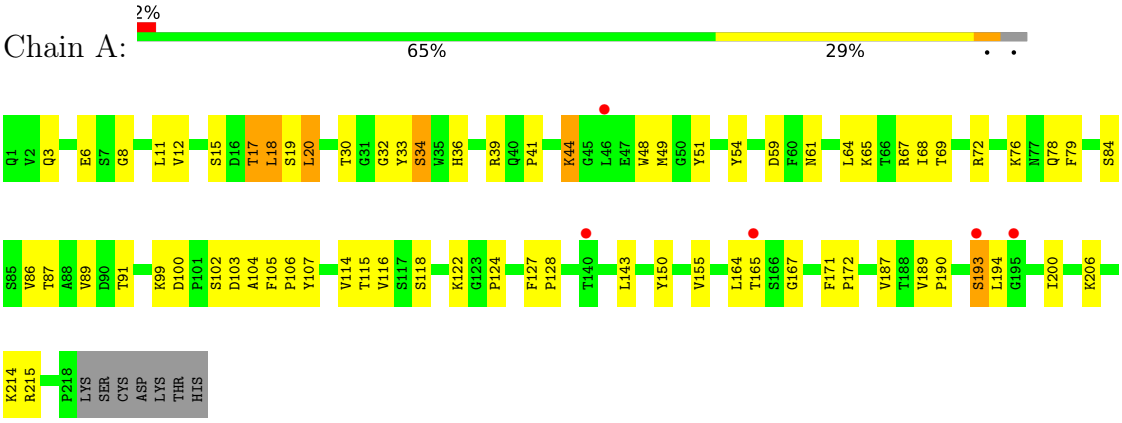
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	35	35	35	0	0
			Total	O		
3	B	25	25	25	0	0
			Total	O		
3	C	29	29	29	0	0
			Total	O		
3	D	23	23	23	0	0
			Total	O		
3	E	18	18	18	0	0
			Total	O		
3	F	22	22	22	0	0
			Total	O		
3	G	42	42	42	0	0
			Total	O		
3	H	21	21	21	0	0
			Total	O		
3	I	37	37	37	0	0
			Total	O		
3	J	28	28	28	0	0
			Total	O		
3	K	33	33	33	0	0
			Total	O		
3	L	24	24	24	0	0
			Total	O		
3	M	29	29	29	0	0
			Total	O		
3	N	32	32	32	0	0
			Total	O		
3	O	19	19	19	0	0
			Total	O		
3	P	26	26	26	0	0

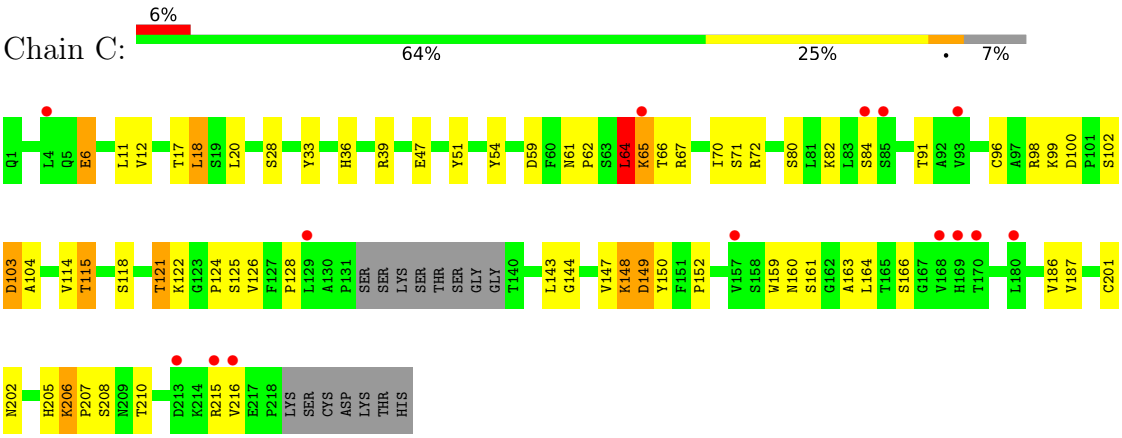
3 Residue-property plots (i)

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

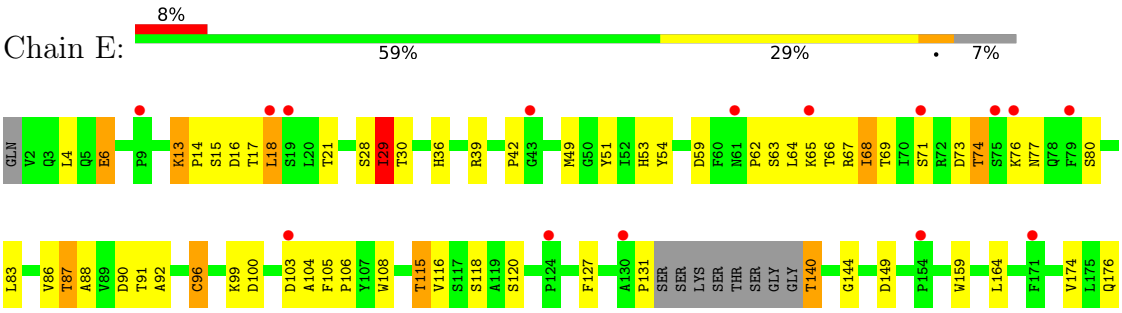
• Molecule 1: Fab Hu 15C1 Heavy chain

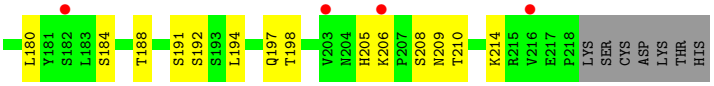


• Molecule 1: Fab Hu 15C1 Heavy chain



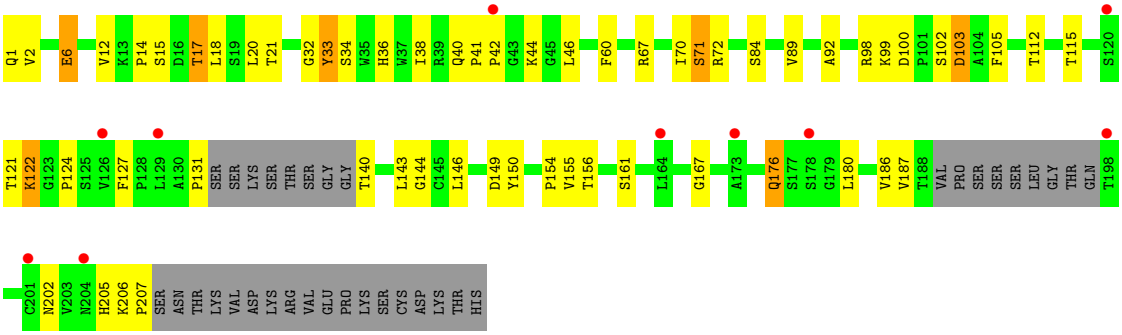
• Molecule 1: Fab Hu 15C1 Heavy chain





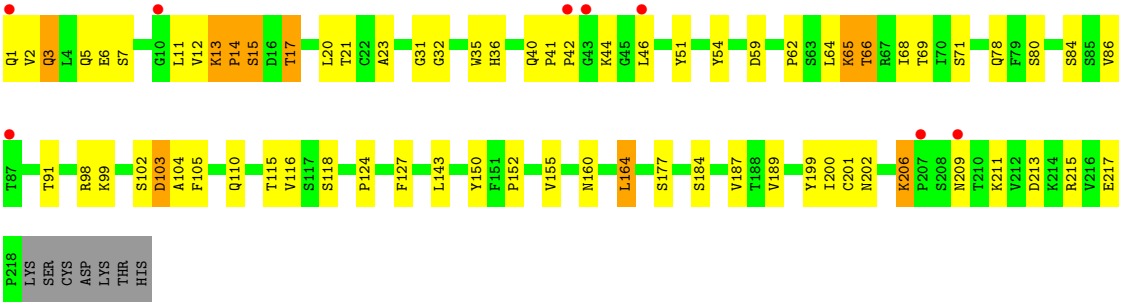
• Molecule 1: Fab Hu 15C1 Heavy chain

Chain G:



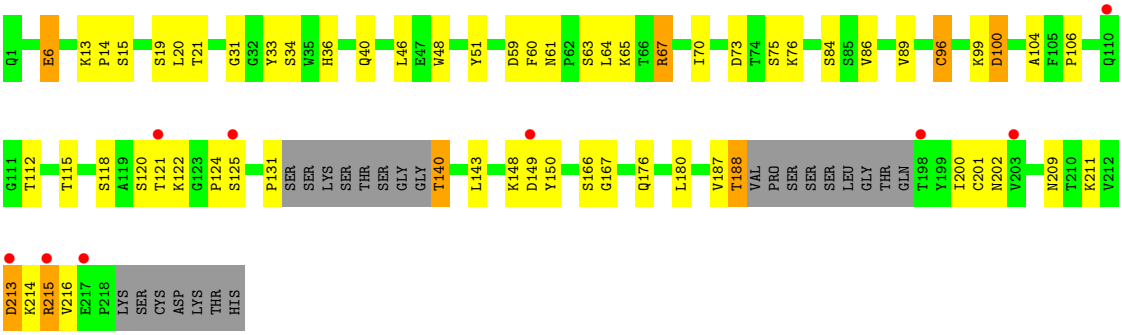
• Molecule 1: Fab Hu 15C1 Heavy chain

Chain I:



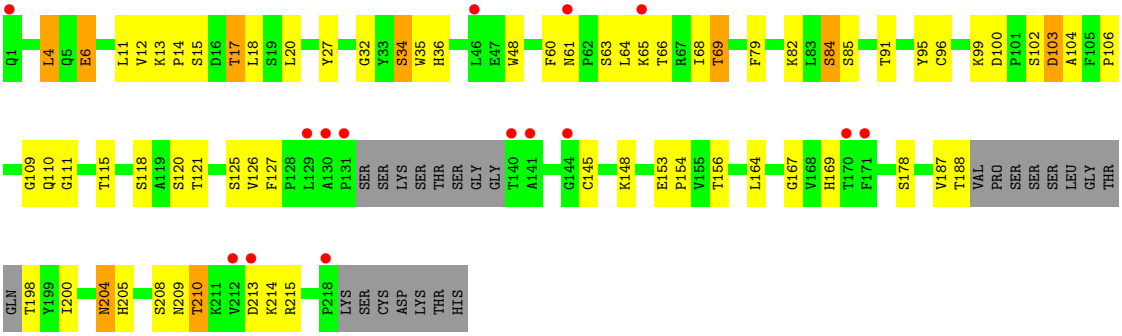
• Molecule 1: Fab Hu 15C1 Heavy chain

Chain K:



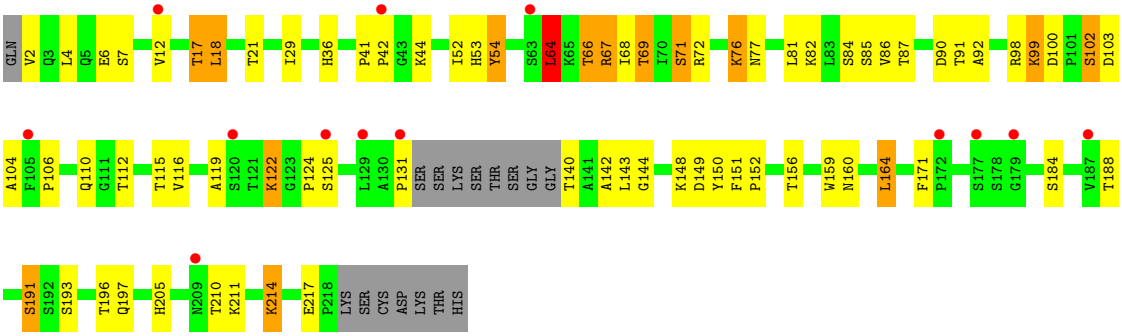
• Molecule 1: Fab Hu 15C1 Heavy chain

Chain M:



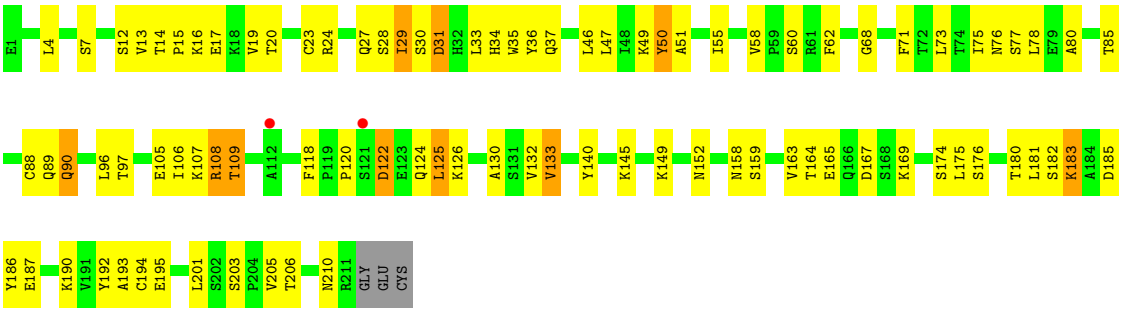
- Molecule 1: Fab Hu 15C1 Heavy chain

Chain O:



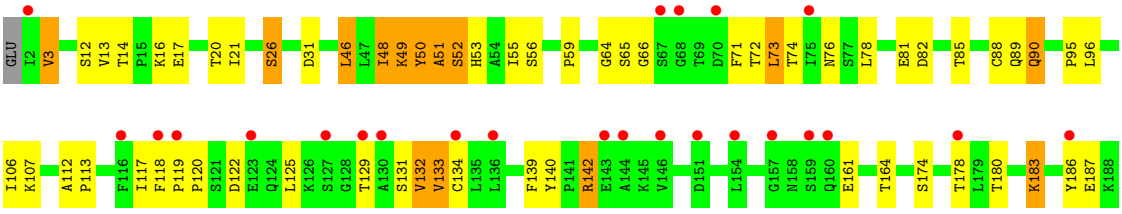
- Molecule 2: Fab Hu 15C1 Light chain

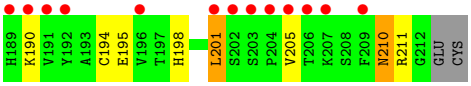
Chain B:



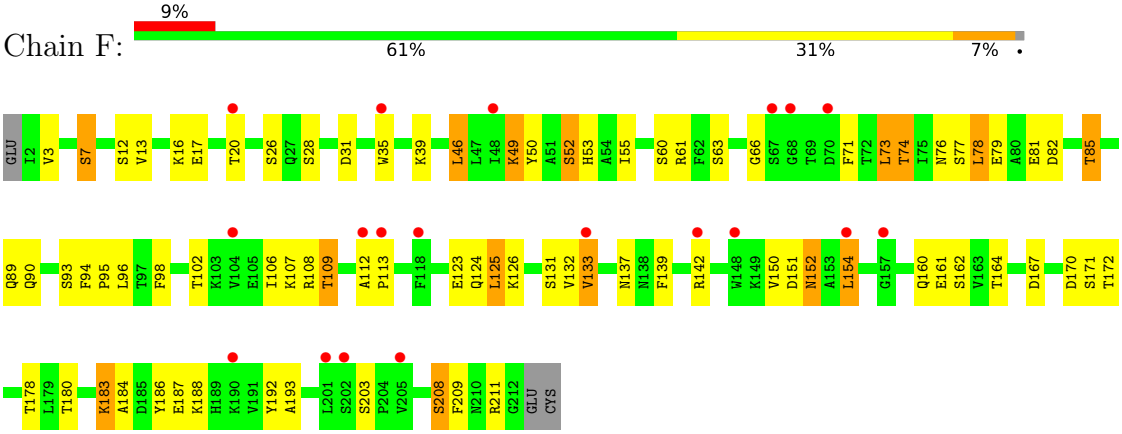
- Molecule 2: Fab Hu 15C1 Light chain

Chain D:

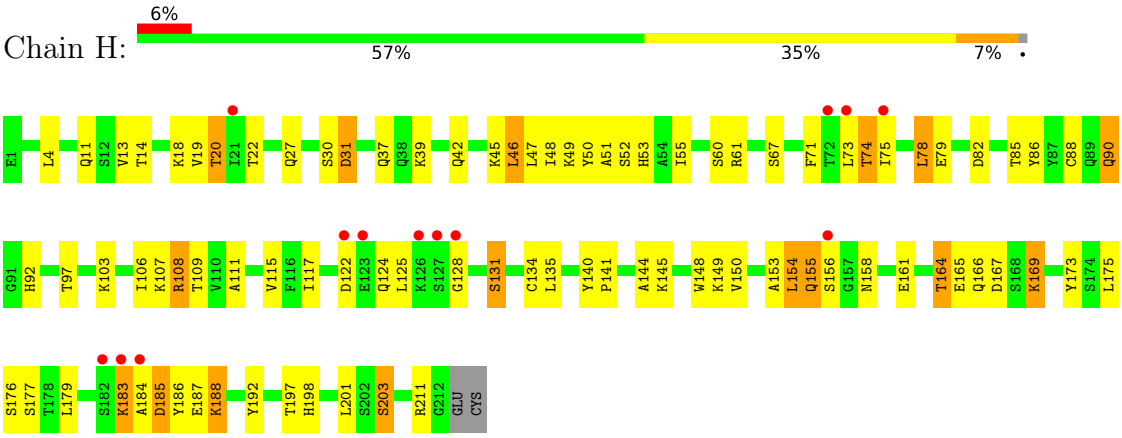




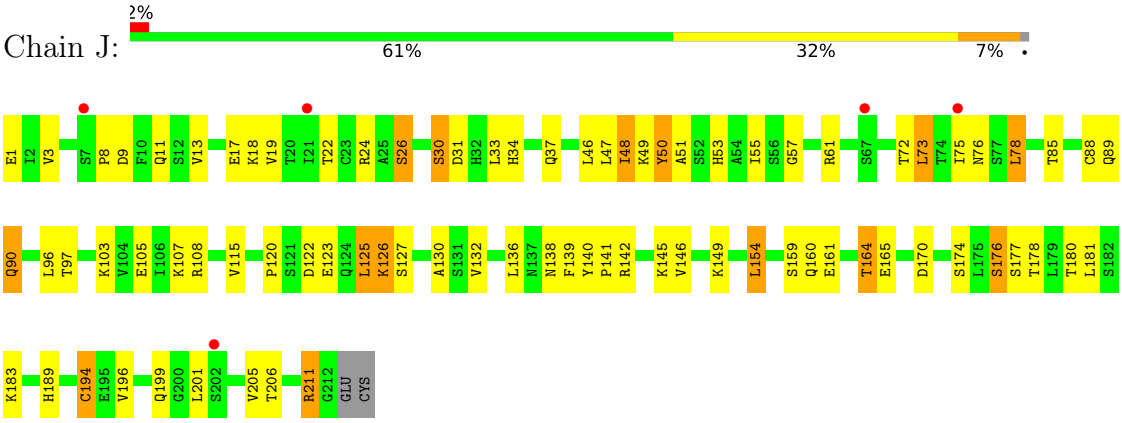
• Molecule 2: Fab Hu 15C1 Light chain



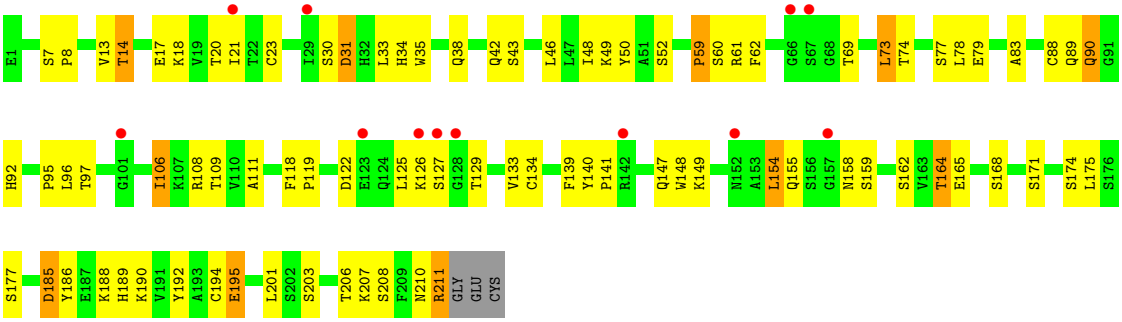
• Molecule 2: Fab Hu 15C1 Light chain



• Molecule 2: Fab Hu 15C1 Light chain

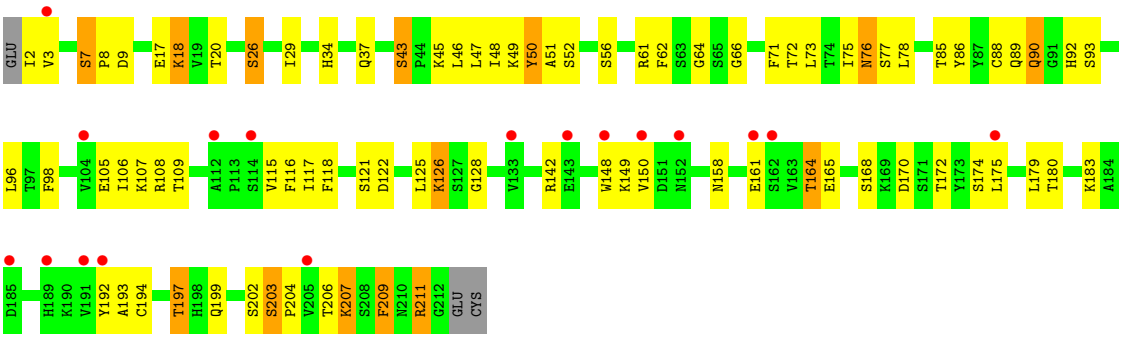


• Molecule 2: Fab Hu 15C1 Light chain



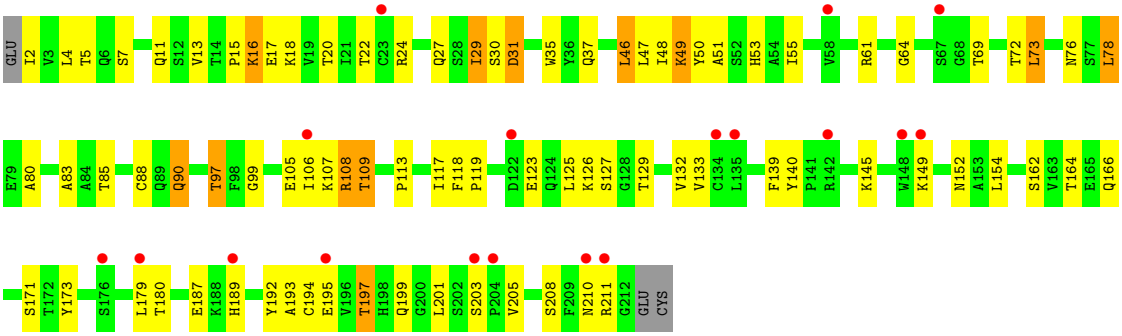
- Molecule 2: Fab Hu 15C1 Light chain

Chain N:



- Molecule 2: Fab Hu 15C1 Light chain

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.82Å 82.51Å 261.57Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75 49.74 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.75) 98.8 (49.74-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.177 , 0.209 0.179 , 0.207	Depositor DCC
R_{free} test set	5475 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 6.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26033	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.58	0/1687	0.68	0/2307
1	C	0.50	0/1638	0.66	1/2241 (0.0%)
1	E	0.50	0/1629	0.69	1/2229 (0.0%)
1	G	0.55	1/1487 (0.1%)	0.69	1/2034 (0.0%)
1	I	0.57	0/1687	0.72	1/2307 (0.0%)
1	K	0.56	0/1576	0.72	2/2154 (0.1%)
1	M	0.49	0/1576	0.66	0/2154
1	O	0.50	0/1629	0.67	0/2229
2	B	0.48	0/1668	0.64	0/2265
2	D	0.47	0/1663	0.66	1/2258 (0.0%)
2	F	0.44	0/1663	0.63	0/2258
2	H	0.46	0/1672	0.64	1/2270 (0.0%)
2	J	0.64	0/1672	0.74	0/2270
2	L	0.48	0/1668	0.64	0/2265
2	N	0.53	0/1663	0.69	0/2258
2	P	0.48	0/1663	0.67	0/2258
All	All	0.52	1/26241 (0.0%)	0.67	8/35757 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	O	0	1
2	D	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	33	TYR	CE1-CZ	-5.35	1.31	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	18	LEU	CA-CB-CG	6.80	130.95	115.30
2	H	31	ASP	CB-CG-OD1	5.92	123.62	118.30
1	K	13	LYS	C-N-CD	5.85	140.68	128.40
1	E	13	LYS	C-N-CD	5.73	140.44	128.40
2	D	52	SER	N-CA-C	5.72	126.43	111.00
1	I	13	LYS	C-N-CD	5.65	140.27	128.40
1	K	31	GLY	N-CA-C	5.38	126.55	113.10
1	C	64	LEU	CA-CB-CG	-5.20	103.35	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	64	LEU	Peptide
2	D	50	TYR	Peptide
2	D	51	ALA	Peptide
1	O	64	LEU	Peptide

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	1641	0	1609	44	0
1	C	1593	0	1562	38	0
1	E	1584	0	1551	46	0
1	G	1445	0	1409	29	0
1	I	1641	0	1609	43	0
1	K	1533	0	1501	34	0
1	M	1533	0	1501	38	0
1	O	1584	0	1551	44	0
2	B	1631	0	1586	47	0
2	D	1626	0	1580	45	0
2	F	1626	0	1580	46	0
2	H	1635	0	1589	52	0
2	J	1635	0	1587	66	0
2	L	1631	0	1586	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1626	0	1580	54	0
2	P	1626	0	1580	50	1
3	A	35	0	0	4	0
3	B	25	0	0	2	0
3	C	29	0	0	3	0
3	D	23	0	0	4	0
3	E	18	0	0	4	0
3	F	22	0	0	4	0
3	G	42	0	0	4	0
3	H	21	0	0	4	1
3	I	37	0	0	4	0
3	J	28	0	0	6	0
3	K	33	0	0	5	0
3	L	24	0	0	4	0
3	M	29	0	0	3	0
3	N	32	0	0	6	0
3	O	19	0	0	6	0
3	P	26	0	0	4	0
All	All	26033	0	24961	698	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (698) 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:E:28:SER:O	1:E:77:ASN:ND2	1.65	1.30
1:O:149:ASP:OD2	3:O:304:HOH:O	1.76	1.04
1:M:6:GLU:OE2	1:M:109:GLY:HA3	1.66	0.96
1:I:32:GLY:HA3	1:I:54:TYR:HB3	1.48	0.95
1:O:99:LYS:HD2	1:O:103:ASP:HB2	1.45	0.95
1:A:41:PRO:HB2	1:A:44:LYS:HG3	1.48	0.93
1:I:127:PHE:CD1	2:J:123:GLU:OE1	2.22	0.92
2:J:31:ASP:OD1	2:J:50:TYR:O	1.85	0.92
2:N:34:HIS:ND1	2:N:49:LYS:O	2.02	0.91
1:O:64:LEU:O	1:O:66:THR:N	2.04	0.90
1:G:176:GLN:NE2	1:G:180:LEU:O	2.06	0.89
1:O:91:THR:HG23	1:O:115:THR:HA	1.52	0.88
2:J:122:ASP:O	2:J:126:LYS:HG2	1.73	0.88
2:L:190:LYS:HE2	2:L:210:ASN:HB3	1.53	0.88
1:I:32:GLY:HA3	1:I:54:TYR:CB	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:PRO:O	1:E:15:SER:OG	1.92	0.86
1:G:124:PRO:HB3	1:G:150:TYR:HB3	1.58	0.86
1:E:131:PRO:O	3:E:307:HOH:O	1.94	0.85
2:F:125:LEU:O	2:F:183:LYS:NZ	2.10	0.84
2:N:202:SER:O	3:N:316:HOH:O	1.97	0.83
1:M:6:GLU:OE2	1:M:109:GLY:CA	2.25	0.82
2:H:184:ALA:O	2:H:188:LYS:NZ	2.10	0.82
1:G:131:PRO:HG3	1:G:143:LEU:HB3	1.62	0.82
2:J:24:ARG:NH2	2:N:17:GLU:OE2	2.14	0.81
2:J:105:GLU:OE2	2:J:140:TYR:OH	1.97	0.81
1:K:188:THR:O	3:K:333:HOH:O	1.97	0.81
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.62	0.81
1:K:14:PRO:O	1:K:15:SER:OG	1.98	0.81
2:F:46:LEU:HD13	2:F:55:ILE:HD11	1.61	0.80
1:E:16:ASP:OD2	3:E:311:HOH:O	2.00	0.80
1:I:5:GLN:OE1	3:I:316:HOH:O	1.98	0.80
1:I:127:PHE:CE1	2:J:123:GLU:OE1	2.35	0.80
1:I:127:PHE:HD1	2:J:123:GLU:OE1	1.66	0.79
2:H:49:LYS:O	2:H:53:HIS:HB2	1.82	0.78
2:P:46:LEU:HD13	2:P:55:ILE:HD11	1.66	0.78
1:K:48:TRP:O	1:K:61:ASN:ND2	2.14	0.78
2:D:190:LYS:HD3	2:D:210:ASN:HB3	1.65	0.78
1:G:34:SER:OG	1:G:36:HIS:NE2	2.17	0.78
2:J:170:ASP:OD2	3:J:311:HOH:O	2.03	0.76
2:B:164:THR:HG22	2:B:174:SER:H	1.51	0.76
1:O:2:VAL:N	3:O:309:HOH:O	2.17	0.76
1:I:66:THR:OG1	3:I:317:HOH:O	2.03	0.75
2:J:50:TYR:N	2:J:51:ALA:HA	2.00	0.75
2:J:49:LYS:O	2:J:53:HIS:HB2	1.86	0.74
2:J:30:SER:OG	2:J:31:ASP:N	2.14	0.74
1:A:34:SER:HB3	1:A:36:HIS:HE2	1.51	0.74
2:D:187:GLU:O	2:D:211:ARG:NH2	2.19	0.74
1:E:87:THR:OG1	1:E:90:ASP:OD2	2.04	0.74
1:I:23:ALA:HA	1:I:78:GLN:HG2	1.68	0.74
1:M:4:LEU:N	1:M:4:LEU:HD12	2.02	0.74
2:P:50:TYR:OH	3:P:301:HOH:O	2.05	0.74
2:F:108:ARG:NH1	2:F:109:THR:O	2.20	0.73
2:L:59:PRO:O	3:L:304:HOH:O	2.06	0.73
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.70	0.73
2:D:142:ARG:NH2	3:D:310:HOH:O	2.22	0.73
1:K:34:SER:OG	1:K:36:HIS:NE2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:171:SER:OG	3:L:306:HOH:O	2.06	0.73
1:O:68:ILE:HD11	1:O:81:LEU:CD1	2.19	0.72
1:A:64:LEU:O	1:A:68:ILE:HG22	1.89	0.72
2:N:128:GLY:HA2	2:N:183:LYS:HD2	1.71	0.72
1:A:18:LEU:HD21	1:A:114:VAL:HG21	1.72	0.72
2:D:13:VAL:O	2:D:107:LYS:N	2.22	0.72
2:B:4:LEU:O	3:B:315:HOH:O	2.08	0.71
2:L:147:GLN:HB3	2:L:195:GLU:HB3	1.71	0.71
1:A:34:SER:HB3	1:A:36:HIS:NE2	2.06	0.71
2:N:149:LYS:HB2	2:N:193:ALA:HB3	1.71	0.70
2:P:2:ILE:N	3:P:317:HOH:O	2.22	0.70
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.73	0.70
1:I:40:GLN:HB2	1:I:46:LEU:HD23	1.74	0.70
2:J:90:GLN:NE2	2:J:97:THR:OG1	2.25	0.70
2:D:48:ILE:HG23	2:D:53:HIS:O	1.91	0.69
1:C:124:PRO:HD2	1:C:210:THR:HG21	1.73	0.69
2:H:188:LYS:HB2	2:H:188:LYS:HZ2	1.57	0.69
2:J:136:LEU:HD11	2:J:196:VAL:HG21	1.73	0.69
2:D:95:PRO:O	3:D:301:HOH:O	2.09	0.69
1:M:60:PHE:HB2	1:M:65:LYS:HD2	1.75	0.69
1:C:54:TYR:O	1:C:72:ARG:NH1	2.24	0.69
1:A:8:GLY:HA3	1:A:20:LEU:HD12	1.73	0.69
2:P:61:ARG:O	2:P:76:ASN:ND2	2.23	0.69
2:P:166:GLN:NE2	2:P:171:SER:O	2.26	0.69
2:H:47:LEU:HB3	2:H:48:ILE:HD12	1.74	0.69
1:K:202:ASN:ND2	1:K:213:ASP:OD2	2.26	0.68
2:L:20:THR:HG22	2:L:74:THR:HG22	1.73	0.68
1:A:87:THR:OG1	3:A:303:HOH:O	2.10	0.68
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.74	0.68
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.75	0.68
1:M:6:GLU:OE2	1:M:110:GLN:N	2.26	0.68
2:N:78:LEU:HD11	2:N:106:ILE:HG12	1.75	0.68
2:H:185:ASP:HA	2:H:188:LYS:HZ3	1.57	0.67
2:D:48:ILE:HG21	2:D:51:ALA:CB	2.24	0.67
1:K:120:SER:O	3:K:302:HOH:O	2.11	0.67
1:E:91:THR:HG23	1:E:115:THR:HA	1.76	0.67
2:L:108:ARG:NH1	2:L:109:THR:O	2.27	0.67
1:G:149:ASP:OD1	3:G:327:HOH:O	2.12	0.67
1:I:41:PRO:HB2	1:I:44:LYS:HD2	1.76	0.67
1:I:64:LEU:O	1:I:68:ILE:HG22	1.95	0.66
1:O:71:SER:OG	3:O:314:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:61:ARG:NH2	3:J:322:HOH:O	2.28	0.66
1:K:104:ALA:O	1:K:106:PRO:HD3	1.96	0.66
2:J:57:GLY:O	3:J:317:HOH:O	2.13	0.66
1:E:42:PRO:HD3	1:E:92:ALA:HA	1.76	0.66
1:C:128:PRO:HB2	1:C:216:VAL:HG13	1.77	0.66
1:O:131:PRO:O	3:O:302:HOH:O	2.13	0.66
2:D:78:LEU:HD11	2:D:106:ILE:HD12	1.77	0.66
2:H:52:SER:HB2	2:H:53:HIS:ND1	2.11	0.66
1:E:140:THR:N	3:E:313:HOH:O	2.29	0.66
2:J:138:ASN:OD1	3:J:314:HOH:O	2.13	0.66
2:P:108:ARG:NH2	3:P:310:HOH:O	2.29	0.66
1:C:144:GLY:HA3	1:C:186:VAL:HG12	1.78	0.65
2:F:133:VAL:HG12	2:F:178:THR:HG23	1.78	0.65
1:C:100:ASP:OD2	3:C:303:HOH:O	2.14	0.65
2:D:133:VAL:HG12	2:D:178:THR:HG23	1.78	0.65
1:K:6:GLU:HG3	1:K:112:THR:HG22	1.78	0.65
1:O:4:LEU:O	3:O:303:HOH:O	2.14	0.65
2:F:78:LEU:HD13	2:F:106:ILE:HG13	1.78	0.65
2:L:139:PHE:HZ	2:L:175:LEU:HB2	1.61	0.65
1:E:86:VAL:HG11	1:E:116:VAL:HG21	1.77	0.65
1:M:120:SER:OG	3:M:308:HOH:O	2.13	0.65
1:O:69:THR:HG23	1:O:82:LYS:HB3	1.79	0.65
2:H:39:LYS:NZ	3:H:321:HOH:O	2.15	0.65
2:J:49:LYS:O	2:J:50:TYR:HB2	1.97	0.64
2:N:197:THR:HG23	2:N:204:PRO:HG3	1.78	0.64
1:M:85:SER:OG	3:M:309:HOH:O	2.15	0.64
2:H:124:GLN:HE22	2:H:131:SER:HB2	1.61	0.64
2:L:33:LEU:HD21	2:L:88:CYS:SG	2.38	0.64
2:N:61:ARG:HD2	2:N:77:SER:HB3	1.78	0.64
2:J:189:HIS:O	2:J:211:ARG:NE	2.25	0.64
2:F:98:PHE:O	3:F:304:HOH:O	2.15	0.64
1:C:6:GLU:OE1	1:C:96:CYS:N	2.31	0.63
1:A:15:SER:O	3:A:329:HOH:O	2.16	0.63
2:H:108:ARG:HD3	2:H:109:THR:O	1.98	0.63
1:A:30:THR:HG22	1:A:72:ARG:NH1	2.14	0.63
1:A:51:TYR:CE1	1:A:59:ASP:HB3	2.34	0.62
2:P:80:ALA:HA	2:P:106:ILE:HD13	1.80	0.62
1:A:72:ARG:NH1	3:A:301:HOH:O	2.32	0.62
1:C:206:LYS:O	1:C:208:SER:HA	1.99	0.62
1:M:6:GLU:OE2	1:M:109:GLY:C	2.36	0.62
2:D:49:LYS:O	2:D:50:TYR:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:TYR:HB2	2:F:53:HIS:HD2	1.64	0.62
1:K:131:PRO:HG3	1:K:143:LEU:HB3	1.81	0.62
1:G:99:LYS:HD2	1:G:103:ASP:HB3	1.80	0.62
1:M:204:ASN:ND2	1:M:210:THR:O	2.33	0.62
2:F:61:ARG:NH2	2:F:82:ASP:OD1	2.33	0.62
2:H:108:ARG:NH1	2:H:111:ALA:HB2	2.15	0.62
2:H:30:SER:OG	2:H:31:ASP:N	2.33	0.62
2:J:48:ILE:HG21	2:J:51:ALA:O	2.00	0.62
1:C:102:SER:HB2	1:C:104:ALA:H	1.63	0.62
2:F:154:LEU:HB2	2:L:154:LEU:HB2	1.81	0.62
1:E:86:VAL:HG12	1:E:87:THR:N	2.15	0.62
2:N:89:GLN:HG3	2:N:98:PHE:CE2	2.34	0.61
1:I:99:LYS:HB2	1:I:105:PHE:CE1	2.35	0.61
2:J:61:ARG:O	2:J:76:ASN:ND2	2.34	0.61
2:J:149:LYS:HG2	2:J:154:LEU:HD22	1.82	0.61
1:A:200:ILE:HD11	1:A:215:ARG:HD3	1.83	0.61
1:G:205:HIS:CD2	1:G:207:PRO:HD2	2.36	0.61
1:E:99:LYS:HE2	1:E:103:ASP:HA	1.83	0.61
1:I:14:PRO:HG3	1:I:116:VAL:HG12	1.82	0.61
1:O:102:SER:N	1:O:103:ASP:HA	2.15	0.61
1:G:155:VAL:HG22	1:G:205:HIS:HB2	1.83	0.61
1:A:102:SER:HB2	1:A:104:ALA:N	2.16	0.60
2:H:46:LEU:HD13	2:H:55:ILE:HD11	1.83	0.60
2:L:201:LEU:O	3:L:313:HOH:O	2.17	0.60
2:P:4:LEU:HD11	2:P:90:GLN:HB2	1.82	0.60
2:B:80:ALA:HA	2:B:106:ILE:HD12	1.83	0.60
2:N:2:ILE:N	3:N:309:HOH:O	2.34	0.60
1:G:102:SER:N	1:G:103:ASP:HA	2.17	0.60
1:I:1:GLN:OE1	1:I:3:GLN:NE2	2.35	0.60
1:O:68:ILE:HD11	1:O:81:LEU:HD12	1.83	0.60
2:F:50:TYR:HB2	2:F:53:HIS:CD2	2.37	0.60
2:F:170:ASP:OD2	2:F:172:THR:OG1	2.20	0.60
2:B:49:LYS:HG3	2:B:55:ILE:HD11	1.84	0.59
1:E:86:VAL:HG13	1:E:90:ASP:HB2	1.84	0.59
2:L:186:TYR:O	2:L:192:TYR:OH	2.19	0.59
1:E:86:VAL:HG13	1:E:90:ASP:CB	2.32	0.59
1:O:68:ILE:CD1	1:O:81:LEU:CD1	2.81	0.59
1:G:60:PHE:HE2	1:G:70:ILE:HG13	1.67	0.59
2:F:112:ALA:O	3:F:312:HOH:O	2.16	0.59
1:E:28:SER:O	1:E:29:ILE:HG22	2.03	0.59
1:O:54:TYR:O	1:O:72:ARG:NH1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:VAL:CG1	1:E:116:VAL:HG21	2.33	0.59
2:N:90:GLN:O	2:N:90:GLN:NE2	2.36	0.58
1:E:208:SER:OG	1:E:210:THR:OG1	2.18	0.58
1:M:34:SER:HB3	1:M:36:HIS:HE2	1.68	0.58
2:H:125:LEU:HD12	2:H:183:LYS:HE3	1.84	0.58
2:P:187:GLU:O	2:P:211:ARG:NH2	2.35	0.58
2:D:59:PRO:O	3:D:313:HOH:O	2.16	0.58
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.86	0.58
2:N:50:TYR:C	2:N:52:SER:H	2.06	0.58
2:P:30:SER:OG	2:P:31:ASP:N	2.35	0.58
1:A:102:SER:HB2	1:A:104:ALA:H	1.69	0.58
2:D:113:PRO:HD3	2:D:198:HIS:ND1	2.19	0.58
1:C:102:SER:N	1:C:103:ASP:HA	2.18	0.57
2:B:14:THR:O	2:B:17:GLU:HB2	2.04	0.57
2:N:161:GLU:HG2	2:N:175:LEU:HD21	1.86	0.57
1:O:131:PRO:HG3	1:O:143:LEU:HB3	1.86	0.57
2:F:113:PRO:HB3	2:F:139:PHE:CD2	2.40	0.57
2:B:29:ILE:C	2:B:30:SER:HG	2.07	0.57
2:B:30:SER:H	2:B:68:GLY:HA2	1.69	0.57
2:F:13:VAL:O	2:F:107:LYS:N	2.31	0.57
2:H:18:LYS:NZ	3:H:305:HOH:O	2.37	0.57
2:N:3:VAL:H	2:N:26:SER:HB2	1.70	0.57
2:B:90:GLN:NE2	2:B:97:THR:OG1	2.34	0.57
2:N:150:VAL:HG22	2:N:192:TYR:CD2	2.40	0.57
1:M:102:SER:N	1:M:103:ASP:HA	2.20	0.57
1:I:124:PRO:HB3	1:I:150:TYR:HB3	1.87	0.56
1:A:30:THR:HG22	1:A:72:ARG:HH12	1.69	0.56
2:J:123:GLU:O	2:J:126:LYS:HG3	2.06	0.56
2:F:89:GLN:HB2	2:F:98:PHE:CE1	2.41	0.56
2:J:33:LEU:O	2:J:51:ALA:HB2	2.06	0.56
1:O:142:ALA:HB2	1:O:188:THR:HG22	1.86	0.56
1:C:102:SER:HB2	1:C:104:ALA:N	2.20	0.56
2:H:49:LYS:HG3	2:H:55:ILE:HD11	1.87	0.56
2:P:108:ARG:NH1	2:P:109:THR:HG22	2.21	0.56
2:F:12:SER:O	3:F:302:HOH:O	2.17	0.55
1:G:72:ARG:NH1	3:G:307:HOH:O	2.32	0.55
2:L:149:LYS:HG2	2:L:154:LEU:HD22	1.87	0.55
1:M:91:THR:HG23	1:M:115:THR:HA	1.89	0.55
1:E:62:PRO:HA	1:E:65:LYS:HB2	1.89	0.55
2:H:103:LYS:NZ	3:H:307:HOH:O	2.26	0.55
2:J:115:VAL:HG22	2:J:136:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:PRO:O	1:I:15:SER:HB3	2.07	0.55
2:J:48:ILE:HD13	2:J:73:LEU:HD23	1.88	0.55
1:K:140:THR:N	3:K:305:HOH:O	2.40	0.55
2:B:108:ARG:HD3	2:B:109:THR:O	2.07	0.55
1:C:18:LEU:HD11	1:C:114:VAL:HG11	1.88	0.55
2:F:193:ALA:HB2	2:F:208:SER:HB3	1.89	0.55
2:N:170:ASP:OD1	2:N:172:THR:OG1	2.23	0.55
1:O:12:VAL:HG11	1:O:18:LEU:HD23	1.89	0.55
1:C:215:ARG:NH2	3:C:310:HOH:O	2.40	0.54
2:B:13:VAL:HG21	2:B:19:VAL:HG22	1.89	0.54
2:H:185:ASP:HA	2:H:188:LYS:NZ	2.21	0.54
1:I:14:PRO:HG3	1:I:116:VAL:CG1	2.37	0.54
2:D:48:ILE:CG2	2:D:51:ALA:CB	2.85	0.54
1:I:102:SER:HB2	1:I:104:ALA:H	1.72	0.54
2:H:186:TYR:O	2:H:192:TYR:OH	2.26	0.54
2:J:122:ASP:O	2:J:126:LYS:CG	2.51	0.54
1:M:104:ALA:O	1:M:106:PRO:HD3	2.06	0.54
1:M:167:GLY:O	1:M:187:VAL:HA	2.07	0.54
2:N:43:SER:OG	3:N:303:HOH:O	2.19	0.54
2:L:49:LYS:HB3	2:L:50:TYR:CD2	2.43	0.54
2:B:164:THR:HG23	2:B:165:GLU:O	2.08	0.54
1:C:11:LEU:HB2	1:C:152:PRO:HG3	1.89	0.54
2:B:186:TYR:O	2:B:192:TYR:OH	2.24	0.54
2:H:39:LYS:O	2:H:42:GLN:HB2	2.07	0.54
2:H:78:LEU:HD13	2:H:106:ILE:HG13	1.90	0.54
2:J:164:THR:HG22	2:J:174:SER:H	1.73	0.54
1:E:105:PHE:O	1:E:108:TRP:NE1	2.41	0.53
1:O:140:THR:N	1:O:191:SER:HG	2.06	0.53
1:A:17:THR:HB	1:A:84:SER:HA	1.89	0.53
1:G:6:GLU:HG3	1:G:112:THR:HG22	1.90	0.53
2:J:48:ILE:CG2	2:J:51:ALA:O	2.55	0.53
2:B:118:PHE:HD2	2:B:133:VAL:HG22	1.74	0.53
2:D:164:THR:HG22	2:D:174:SER:H	1.72	0.53
1:K:36:HIS:CE1	1:K:51:TYR:HB3	2.44	0.53
2:J:125:LEU:HD11	2:J:130:ALA:HB2	1.90	0.53
2:P:90:GLN:NE2	2:P:97:THR:OG1	2.41	0.53
1:C:36:HIS:CE1	1:C:51:TYR:HB3	2.43	0.53
2:D:117:ILE:HD12	2:D:194:CYS:HB2	1.91	0.53
1:M:34:SER:HB3	1:M:36:HIS:NE2	2.24	0.53
2:B:122:ASP:OD1	2:B:126:LYS:NZ	2.34	0.52
1:G:2:VAL:HG21	1:G:98:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:GLU:HB3	1:K:118:SER:HB3	1.90	0.52
2:N:122:ASP:O	2:N:126:LYS:HD2	2.09	0.52
1:C:148:LYS:O	1:C:149:ASP:HB2	2.09	0.52
2:J:115:VAL:HG22	2:J:136:LEU:CD1	2.39	0.52
1:E:149:ASP:O	1:E:180:LEU:HD13	2.09	0.52
1:I:17:THR:HG22	3:I:303:HOH:O	2.10	0.52
2:N:90:GLN:HE22	2:N:96:LEU:HA	1.75	0.52
1:O:151:PHE:CD1	1:O:152:PRO:HA	2.44	0.52
2:D:190:LYS:O	2:D:210:ASN:HA	2.09	0.52
1:E:64:LEU:O	1:E:68:ILE:HG22	2.10	0.52
1:E:68:ILE:HG12	1:E:69:THR:N	2.23	0.52
2:H:128:GLY:HA2	2:H:183:LYS:HB3	1.90	0.52
2:J:49:LYS:C	2:J:51:ALA:HA	2.30	0.52
1:C:11:LEU:HD23	1:C:121:THR:HG22	1.92	0.52
1:G:89:VAL:O	3:G:313:HOH:O	2.18	0.52
1:C:65:LYS:N	1:C:66:THR:HA	2.25	0.52
2:F:184:ALA:O	2:F:188:LYS:HG3	2.10	0.51
1:G:14:PRO:O	1:G:15:SER:OG	2.27	0.51
2:J:164:THR:HG23	2:J:165:GLU:O	2.09	0.51
1:I:91:THR:O	3:I:310:HOH:O	2.19	0.51
2:D:48:ILE:HG21	2:D:51:ALA:HB1	1.92	0.51
1:E:99:LYS:HB2	1:E:105:PHE:CE2	2.46	0.51
1:O:193:SER:HB2	1:O:197:GLN:HG2	1.90	0.51
1:E:28:SER:OG	1:E:29:ILE:N	2.43	0.51
2:H:11:GLN:HE21	2:H:19:VAL:HG13	1.75	0.51
2:J:11:GLN:HG3	2:N:8:PRO:HG3	1.90	0.51
1:K:19:SER:OG	3:K:317:HOH:O	2.19	0.51
1:K:33:TYR:CZ	3:K:331:HOH:O	2.54	0.51
2:N:158:ASN:ND2	2:N:179:LEU:HD11	2.25	0.51
2:F:13:VAL:HG13	2:F:17:GLU:HB3	1.92	0.51
2:H:19:VAL:HB	2:H:75:ILE:HB	1.93	0.51
2:F:61:ARG:HH21	2:F:82:ASP:CG	2.14	0.51
1:M:153:GLU:OE2	1:M:154:PRO:HA	2.11	0.51
2:P:47:LEU:HB3	2:P:48:ILE:HD12	1.92	0.51
1:K:99:LYS:HE3	1:K:100:ASP:O	2.10	0.51
1:A:32:GLY:O	1:A:33:TYR:HB2	2.10	0.51
1:E:86:VAL:HG11	1:E:116:VAL:CG2	2.41	0.51
2:H:45:LYS:NZ	3:H:321:HOH:O	2.44	0.51
2:B:158:ASN:N	2:B:158:ASN:OD1	2.43	0.51
1:I:31:GLY:N	1:I:32:GLY:HA2	2.25	0.51
2:D:107:LYS:HA	2:D:140:TYR:OH	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:HA2	1:A:54:TYR:CD2	2.45	0.50
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.26	0.50
2:N:50:TYR:O	2:N:52:SER:N	2.44	0.50
2:N:203:SER:O	3:N:317:HOH:O	2.18	0.50
2:P:193:ALA:HB2	2:P:208:SER:HB3	1.92	0.50
1:A:102:SER:N	1:A:103:ASP:HA	2.26	0.50
2:L:50:TYR:O	2:L:52:SER:N	2.41	0.50
1:M:48:TRP:O	1:M:61:ASN:ND2	2.40	0.50
2:F:187:GLU:O	2:F:211:ARG:NH2	2.45	0.50
2:J:30:SER:HG	2:J:31:ASP:H	1.53	0.50
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.47	0.50
2:N:108:ARG:NH1	2:N:109:THR:O	2.44	0.50
1:C:91:THR:HG23	1:C:115:THR:HA	1.94	0.50
1:G:42:PRO:HD3	1:G:92:ALA:HA	1.93	0.50
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.94	0.50
2:J:17:GLU:OE1	2:N:7:SER:OG	2.30	0.49
2:L:158:ASN:OD1	2:L:158:ASN:N	2.42	0.49
2:P:201:LEU:HD13	2:P:205:VAL:HG23	1.92	0.49
2:D:48:ILE:CG2	2:D:51:ALA:HB2	2.42	0.49
2:H:149:LYS:HA	2:H:153:ALA:O	2.12	0.49
2:N:148:TRP:CE2	2:N:179:LEU:HB2	2.47	0.49
1:C:70:ILE:HG23	1:C:80:SER:O	2.13	0.49
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.94	0.49
2:N:92:HIS:HD2	2:N:93:SER:HB2	1.78	0.49
1:O:68:ILE:CD1	1:O:81:LEU:HD12	2.42	0.49
2:B:30:SER:OG	2:B:31:ASP:N	2.42	0.49
1:A:86:VAL:HG12	1:A:116:VAL:HG11	1.94	0.49
1:E:127:PHE:CE1	2:F:124:GLN:HA	2.48	0.49
2:H:201:LEU:HB3	2:H:203:SER:O	2.12	0.49
1:K:167:GLY:O	1:K:187:VAL:HA	2.13	0.49
2:P:117:ILE:HD12	2:P:194:CYS:HB2	1.95	0.49
1:A:41:PRO:HB2	1:A:44:LYS:CG	2.34	0.49
2:D:122:ASP:HA	2:D:125:LEU:HB2	1.94	0.49
1:G:41:PRO:HB2	1:G:44:LYS:HD3	1.95	0.49
2:F:49:LYS:O	2:F:53:HIS:HB2	2.12	0.49
2:H:82:ASP:O	2:H:86:TYR:OH	2.20	0.49
1:K:201:CYS:O	1:K:213:ASP:HA	2.13	0.49
1:O:36:HIS:NE2	1:O:99:LYS:HB2	2.28	0.49
2:F:123:GLU:HA	2:F:126:LYS:HG3	1.95	0.48
2:H:13:VAL:HB	2:H:78:LEU:HD12	1.95	0.48
1:K:124:PRO:HB3	1:K:150:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:GLU:OE1	1:M:95:TYR:HA	2.13	0.48
2:B:105:GLU:HG2	2:B:106:ILE:N	2.27	0.48
1:O:102:SER:HB2	1:O:104:ALA:H	1.79	0.48
2:D:64:GLY:HA2	2:D:72:THR:O	2.14	0.48
1:I:99:LYS:HE2	1:I:103:ASP:HB2	1.94	0.48
1:A:106:PRO:HB2	1:A:107:TYR:CD2	2.48	0.48
1:E:21:THR:HA	1:E:80:SER:HA	1.96	0.48
2:H:175:LEU:HD23	2:H:176:SER:N	2.28	0.48
1:I:160:ASN:HB2	1:I:164:LEU:HB2	1.94	0.48
2:B:35:TRP:NE1	3:B:310:HOH:O	2.34	0.48
1:K:6:GLU:OE1	1:K:96:CYS:N	2.47	0.48
1:M:99:LYS:HD2	1:M:103:ASP:HB3	1.96	0.48
2:N:164:THR:HG23	2:N:165:GLU:O	2.13	0.48
2:N:209:PHE:CD1	2:N:209:PHE:C	2.87	0.48
1:C:122:LYS:HG2	1:C:149:ASP:O	2.13	0.48
1:O:87:THR:O	1:O:116:VAL:HG11	2.13	0.48
2:P:13:VAL:HG13	2:P:17:GLU:HB3	1.94	0.48
2:P:113:PRO:HB3	2:P:139:PHE:CD1	2.49	0.48
2:D:31:ASP:O	2:D:50:TYR:HD1	1.96	0.48
2:D:48:ILE:CG2	2:D:51:ALA:HA	2.43	0.48
2:L:164:THR:HG23	2:L:165:GLU:O	2.14	0.48
1:A:99:LYS:HB2	1:A:105:PHE:CE1	2.48	0.48
2:D:66:GLY:HA3	2:D:71:PHE:HA	1.96	0.48
2:J:47:LEU:O	2:J:55:ILE:HG12	2.14	0.48
2:J:107:LYS:HE2	2:J:107:LYS:HB2	1.66	0.48
1:O:193:SER:O	1:O:197:GLN:HG2	2.14	0.48
1:E:18:LEU:N	1:E:83:LEU:O	2.39	0.47
2:J:201:LEU:HD13	2:J:205:VAL:HG23	1.94	0.47
2:L:13:VAL:HG13	2:L:17:GLU:CD	2.34	0.47
2:L:83:ALA:HB2	2:L:106:ILE:HD11	1.96	0.47
1:E:39:ARG:HB3	1:E:49:MET:SD	2.55	0.47
1:E:188:THR:HG21	2:F:137:ASN:ND2	2.28	0.47
2:H:144:ALA:HB2	2:H:198:HIS:HD2	1.79	0.47
1:I:164:LEU:CD1	1:I:187:VAL:HG21	2.44	0.47
1:K:6:GLU:OE1	1:K:96:CYS:HB2	2.13	0.47
2:D:112:ALA:HB1	2:D:201:LEU:HD23	1.96	0.47
1:I:51:TYR:CE1	1:I:59:ASP:HB3	2.49	0.47
2:N:108:ARG:HG3	2:N:109:THR:O	2.14	0.47
1:O:119:ALA:HB3	1:O:151:PHE:CE2	2.49	0.47
2:F:124:GLN:HE22	2:F:131:SER:N	2.12	0.47
2:J:194:CYS:O	2:J:206:THR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:24:ARG:HD3	3:P:320:HOH:O	2.15	0.47
2:P:105:GLU:OE2	2:P:173:TYR:OH	2.20	0.47
1:C:160:ASN:HB2	1:C:163:ALA:HB3	1.96	0.47
1:O:171:PHE:HB3	2:P:162:SER:OG	2.15	0.47
2:B:30:SER:O	2:B:71:PHE:CZ	2.67	0.47
2:F:192:TYR:HB2	2:F:209:PHE:CZ	2.50	0.47
2:F:49:LYS:HG3	2:F:53:HIS:HB2	1.96	0.47
2:F:61:ARG:NH1	3:F:303:HOH:O	2.48	0.47
2:F:66:GLY:HA3	2:F:71:PHE:HA	1.97	0.47
2:H:61:ARG:NE	2:H:82:ASP:OD2	2.41	0.47
2:H:164:THR:HG23	2:H:165:GLU:O	2.15	0.47
1:M:103:ASP:OD1	1:M:103:ASP:N	2.48	0.47
2:N:61:ARG:HA	2:N:61:ARG:HD3	1.62	0.47
1:A:39:ARG:HD3	1:A:49:MET:SD	2.55	0.47
1:I:32:GLY:CA	1:I:54:TYR:HB3	2.31	0.47
2:J:33:LEU:HD22	2:J:89:GLN:O	2.15	0.47
2:L:90:GLN:HG2	2:L:92:HIS:H	1.80	0.47
2:J:19:VAL:HB	2:J:75:ILE:HB	1.97	0.47
2:L:148:TRP:HB2	2:L:155:GLN:HB2	1.96	0.47
1:O:76:LYS:HA	3:O:316:HOH:O	2.15	0.47
2:H:145:LYS:HB3	2:H:197:THR:HB	1.96	0.47
1:M:11:LEU:HD23	1:M:121:THR:HG22	1.97	0.47
2:B:167:ASP:OD1	2:B:169:LYS:N	2.37	0.46
1:C:54:TYR:HA	3:C:308:HOH:O	2.14	0.46
2:N:66:GLY:HA3	2:N:71:PHE:HA	1.97	0.46
2:P:118:PHE:HA	2:P:119:PRO:HD2	1.74	0.46
1:E:174:VAL:HG11	2:F:160:GLN:HB3	1.97	0.46
1:I:189:VAL:HG11	1:I:199:TYR:CE2	2.50	0.46
2:J:1:GLU:N	3:J:305:HOH:O	2.48	0.46
2:J:139:PHE:CD1	2:J:139:PHE:N	2.82	0.46
2:L:33:LEU:HD22	2:L:89:GLN:O	2.15	0.46
2:B:30:SER:HA	2:B:68:GLY:H	1.80	0.46
1:A:11:LEU:HD12	1:A:115:THR:O	2.16	0.46
1:A:99:LYS:HE2	1:A:100:ASP:O	2.16	0.46
2:B:180:THR:O	2:B:181:LEU:HD23	2.15	0.46
2:D:210:ASN:ND2	3:D:311:HOH:O	2.22	0.46
2:H:4:LEU:HD13	2:H:88:CYS:HB3	1.97	0.46
1:I:62:PRO:HA	1:I:65:LYS:HG3	1.96	0.46
1:O:2:VAL:HG21	1:O:98:ARG:NH1	2.31	0.46
1:O:17:THR:HA	1:O:84:SER:HA	1.98	0.46
1:E:86:VAL:CG1	1:E:87:THR:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:ILE:HD11	1:G:105:PHE:CE2	2.50	0.46
2:H:148:TRP:CE2	2:H:179:LEU:HB2	2.51	0.46
1:I:91:THR:HG23	1:I:115:THR:HA	1.97	0.46
2:N:34:HIS:CE1	2:N:49:LYS:O	2.66	0.46
2:P:37:GLN:HB2	2:P:47:LEU:CD1	2.44	0.46
1:E:36:HIS:CE1	1:E:51:TYR:HB3	2.51	0.46
1:M:204:ASN:HD22	1:M:205:HIS:N	2.14	0.46
2:P:27:GLN:O	2:P:29:ILE:HG23	2.15	0.46
1:C:51:TYR:CE1	1:C:59:ASP:HB3	2.51	0.46
1:G:122:LYS:HD2	1:G:180:LEU:HD13	1.97	0.46
2:H:166:GLN:HB2	2:H:173:TYR:CZ	2.50	0.46
2:J:18:LYS:NZ	3:J:301:HOH:O	2.45	0.46
1:M:126:VAL:O	1:M:214:LYS:NZ	2.49	0.46
1:O:68:ILE:HD12	1:O:82:LYS:O	2.16	0.46
1:E:91:THR:O	3:E:309:HOH:O	2.21	0.46
2:H:20:THR:HG23	2:H:74:THR:HG23	1.97	0.46
2:J:8:PRO:HG2	2:J:11:GLN:HB2	1.98	0.46
2:L:38:GLN:HG3	2:L:42:GLN:O	2.15	0.46
2:L:185:ASP:N	2:L:185:ASP:OD1	2.48	0.46
1:M:17:THR:HB	1:M:84:SER:HA	1.97	0.46
1:M:127:PHE:HB3	2:N:121:SER:OG	2.16	0.46
2:N:62:PHE:CE2	2:N:75:ILE:HG12	2.50	0.46
1:O:122:LYS:HD2	1:O:149:ASP:O	2.15	0.46
1:C:103:ASP:OD1	1:C:103:ASP:N	2.49	0.45
2:J:3:VAL:H	2:J:26:SER:HB2	1.82	0.45
1:K:200:ILE:HG12	1:K:215:ARG:HB2	1.98	0.45
1:M:27:TYR:HE2	1:M:32:GLY:HA2	1.81	0.45
2:P:108:ARG:HD3	2:P:109:THR:O	2.17	0.45
2:D:3:VAL:N	2:D:26:SER:OG	2.49	0.45
2:J:78:LEU:HD23	2:J:78:LEU:HA	1.82	0.45
2:N:116:PHE:HA	3:N:315:HOH:O	2.16	0.45
2:D:190:LYS:CD	2:D:210:ASN:HB3	2.42	0.45
1:M:178:SER:OG	3:M:320:HOH:O	2.19	0.45
2:B:125:LEU:O	2:B:183:LYS:NZ	2.30	0.45
1:I:206:LYS:H	1:I:206:LYS:HG3	1.60	0.45
1:O:67:ARG:NH2	1:O:90:ASP:OD1	2.49	0.45
2:H:149:LYS:HG2	2:H:154:LEU:HD22	1.99	0.45
2:J:33:LEU:HD21	2:J:88:CYS:SG	2.57	0.45
1:M:200:ILE:HD13	1:M:215:ARG:HB2	1.98	0.45
1:O:41:PRO:HA	1:O:42:PRO:HD3	1.88	0.45
1:A:127:PHE:CD1	2:B:124:GLN:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:TRP:HB3	1:M:79:PHE:CZ	2.52	0.45
2:N:45:LYS:HB2	2:N:45:LYS:HE3	1.79	0.45
1:A:48:TRP:CE2	2:B:96:LEU:HD13	2.51	0.45
2:J:145:LYS:HG2	2:J:146:VAL:N	2.32	0.45
2:J:159:SER:HA	2:J:178:THR:O	2.17	0.45
2:L:108:ARG:HG3	2:L:109:THR:O	2.16	0.45
1:A:128:PRO:HD3	1:A:214:LYS:HE2	1.99	0.45
2:D:78:LEU:HD11	2:D:106:ILE:CD1	2.47	0.45
2:D:131:SER:OG	2:D:180:THR:HG22	2.17	0.45
1:G:17:THR:HB	1:G:84:SER:HA	1.98	0.45
1:K:148:LYS:HD3	1:K:149:ASP:OD2	2.17	0.45
1:K:200:ILE:HD11	1:K:215:ARG:NH2	2.32	0.45
1:A:17:THR:HG23	3:A:308:HOH:O	2.16	0.45
1:K:60:PHE:HE1	1:K:70:ILE:HG13	1.81	0.45
2:P:4:LEU:HB2	2:P:99:GLY:HA2	1.99	0.45
1:A:99:LYS:HG2	1:A:100:ASP:O	2.17	0.44
1:E:30:THR:HG21	1:E:74:THR:HG22	1.98	0.44
2:F:94:PHE:HA	2:F:95:PRO:C	2.38	0.44
1:I:102:SER:N	1:I:103:ASP:HA	2.32	0.44
2:N:64:GLY:HA2	2:N:72:THR:O	2.17	0.44
1:O:214:LYS:NZ	2:P:123:GLU:OE1	2.45	0.44
2:P:108:ARG:H	2:P:108:ARG:HG3	1.60	0.44
1:A:91:THR:HG23	1:A:115:THR:HA	1.98	0.44
2:D:14:THR:O	2:D:17:GLU:HB3	2.17	0.44
1:E:99:LYS:HG2	1:E:100:ASP:O	2.18	0.44
2:F:193:ALA:CB	2:F:208:SER:HB3	2.47	0.44
2:L:14:THR:O	2:L:17:GLU:HB3	2.18	0.44
2:D:89:GLN:HG2	2:D:90:GLN:N	2.31	0.44
2:H:37:GLN:HG3	2:H:86:TYR:CE2	2.53	0.44
1:I:71:SER:OG	1:I:80:SER:HB2	2.17	0.44
1:M:198:THR:HG21	1:M:215:ARG:NH2	2.33	0.44
2:P:132:VAL:HB	2:P:179:LEU:HB3	2.00	0.44
1:E:53:HIS:CE1	1:E:54:TYR:CE1	3.05	0.44
2:F:73:LEU:HD22	2:F:74:THR:H	1.83	0.44
2:F:85:THR:HA	2:F:102:THR:O	2.17	0.44
1:A:167:GLY:O	1:A:187:VAL:HA	2.17	0.44
2:L:206:THR:O	2:L:207:LYS:HD2	2.16	0.44
1:O:68:ILE:HD12	1:O:69:THR:H	1.82	0.44
2:D:31:ASP:O	2:D:50:TYR:HA	2.18	0.44
2:D:125:LEU:O	2:D:183:LYS:HE3	2.18	0.44
1:K:202:ASN:HD22	1:K:213:ASP:CG	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:194:CYS:O	2:N:206:THR:HA	2.18	0.44
2:P:108:ARG:HG2	2:P:171:SER:HB2	1.99	0.44
2:B:24:ARG:HH21	2:D:17:GLU:HA	1.83	0.44
2:N:117:ILE:HG13	2:N:118:PHE:N	2.32	0.44
1:O:29:ILE:HG23	1:O:77:ASN:OD1	2.18	0.44
2:J:22:THR:HG22	2:J:72:THR:OG1	2.18	0.44
2:P:189:HIS:HB2	2:P:192:TYR:OH	2.18	0.44
2:B:14:THR:HB	2:B:17:GLU:CD	2.38	0.43
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.99	0.43
2:F:63:SER:O	2:F:74:THR:N	2.46	0.43
2:J:140:TYR:CG	2:J:141:PRO:HA	2.53	0.43
2:P:149:LYS:HZ1	2:P:195:GLU:CD	2.20	0.43
2:B:47:LEU:O	2:B:55:ILE:HG12	2.17	0.43
2:L:34:HIS:ND1	2:L:49:LYS:HA	2.32	0.43
1:M:99:LYS:CD	1:M:103:ASP:HB3	2.48	0.43
2:N:18:LYS:HG2	2:N:76:ASN:HA	2.00	0.43
2:B:50:TYR:N	2:B:51:ALA:HA	2.33	0.43
1:E:86:VAL:CG1	1:E:90:ASP:HB2	2.46	0.43
1:M:6:GLU:CD	1:M:111:GLY:H	2.22	0.43
2:P:2:ILE:HB	2:P:90:GLN:NE2	2.32	0.43
2:P:13:VAL:HG12	2:P:78:LEU:HD12	1.98	0.43
2:F:46:LEU:HD13	2:F:55:ILE:CD1	2.41	0.43
1:I:36:HIS:ND1	1:I:51:TYR:HB3	2.33	0.43
2:B:149:LYS:HB2	2:B:193:ALA:HB3	2.01	0.43
1:E:144:GLY:HA2	1:E:159:TRP:CZ2	2.54	0.43
2:L:62:PHE:HD1	3:L:304:HOH:O	2.01	0.43
2:P:46:LEU:HD13	2:P:55:ILE:CD1	2.44	0.43
1:A:104:ALA:O	1:A:106:PRO:HD3	2.19	0.43
1:K:215:ARG:HG3	1:K:216:VAL:N	2.31	0.43
2:P:18:LYS:HG3	2:P:76:ASN:HA	2.00	0.43
2:B:201:LEU:HD13	2:B:205:VAL:HG23	2.01	0.43
2:F:35:TRP:CE2	2:F:73:LEU:HB2	2.53	0.43
2:H:158:ASN:ND2	2:H:179:LEU:HD11	2.34	0.43
2:J:127:SER:O	2:J:127:SER:OG	2.35	0.43
1:A:48:TRP:CE3	1:A:61:ASN:HB2	2.54	0.43
1:E:6:GLU:OE1	1:E:96:CYS:N	2.51	0.43
1:E:205:HIS:HB3	1:E:210:THR:HB	2.00	0.43
1:I:11:LEU:HB2	1:I:152:PRO:HG3	1.99	0.43
1:A:171:PHE:HA	1:A:172:PRO:HD2	1.75	0.43
2:H:11:GLN:HE22	2:H:20:THR:H	1.67	0.43
2:H:115:VAL:HA	2:H:135:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLY:HA3	1:I:54:TYR:HB2	1.95	0.43
1:I:202:ASN:ND2	1:I:213:ASP:OD2	2.51	0.43
2:D:113:PRO:HD2	2:D:201:LEU:HD21	2.00	0.43
2:F:17:GLU:HG2	2:L:7:SER:HB3	2.00	0.43
2:H:90:GLN:HG2	2:H:92:HIS:H	1.84	0.43
2:B:55:ILE:HB	2:B:58:VAL:HG21	2.01	0.42
1:C:124:PRO:HB3	1:C:150:TYR:HB3	1.99	0.42
2:H:50:TYR:O	2:H:51:ALA:HB3	2.19	0.42
1:I:2:VAL:HG21	1:I:98:ARG:NH1	2.34	0.42
2:L:30:SER:O	2:L:30:SER:OG	2.28	0.42
1:O:205:HIS:HB3	1:O:210:THR:HB	2.01	0.42
2:P:83:ALA:HB2	2:P:106:ILE:HD12	1.99	0.42
1:A:36:HIS:ND1	1:A:51:TYR:HB3	2.33	0.42
1:I:36:HIS:CE1	1:I:99:LYS:HD3	2.54	0.42
2:P:149:LYS:HZ2	2:P:195:GLU:HB2	1.84	0.42
1:A:72:ARG:HA	1:A:79:PHE:HA	2.01	0.42
2:B:89:GLN:HG2	2:B:90:GLN:N	2.33	0.42
1:C:67:ARG:HD2	1:C:84:SER:O	2.19	0.42
2:F:151:ASP:O	2:F:152:ASN:HB2	2.19	0.42
2:L:33:LEU:HD13	2:L:34:HIS:N	2.34	0.42
2:N:50:TYR:C	2:N:52:SER:N	2.72	0.42
1:O:124:PRO:HA	1:O:150:TYR:HB3	2.01	0.42
1:A:106:PRO:HB2	1:A:107:TYR:CE2	2.54	0.42
1:C:33:TYR:CE2	1:C:98:ARG:CZ	3.02	0.42
1:C:64:LEU:HA	1:C:64:LEU:HD23	1.75	0.42
1:C:161:SER:H	1:C:202:ASN:ND2	2.17	0.42
1:E:206:LYS:HB3	1:E:206:LYS:HE3	1.56	0.42
2:H:150:VAL:HG12	2:H:155:GLN:OE1	2.19	0.42
2:J:161:GLU:HA	2:J:176:SER:O	2.19	0.42
1:K:51:TYR:CE1	1:K:59:ASP:HB3	2.54	0.42
1:K:67:ARG:HD2	1:K:84:SER:O	2.19	0.42
2:L:21:ILE:HD12	2:L:73:LEU:HD12	2.01	0.42
1:O:144:GLY:HA2	1:O:159:TRP:CZ2	2.55	0.42
2:P:107:LYS:HA	2:P:140:TYR:CZ	2.54	0.42
1:C:99:LYS:NZ	1:C:103:ASP:HB3	2.34	0.42
2:J:34:HIS:O	2:J:89:GLN:N	2.33	0.42
2:J:149:LYS:HG2	2:J:154:LEU:CD2	2.47	0.42
2:B:14:THR:HG23	2:B:15:PRO:HD2	2.01	0.42
2:L:189:HIS:O	2:L:211:ARG:HD3	2.18	0.42
1:C:159:TRP:CZ3	1:C:201:CYS:HB3	2.55	0.42
1:O:160:ASN:HB2	1:O:164:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:64:GLY:HA2	2:P:72:THR:O	2.20	0.42
1:C:61:ASN:HA	1:C:62:PRO:HD3	1.87	0.42
1:G:100:ASP:HB2	1:G:102:SER:OG	2.20	0.42
1:K:40:GLN:HB2	1:K:46:LEU:HD23	2.01	0.42
1:I:41:PRO:HA	1:I:42:PRO:HD3	1.95	0.42
2:B:195:GLU:HG3	2:B:206:THR:OG1	2.20	0.42
1:C:6:GLU:H	1:C:6:GLU:HG2	1.43	0.42
1:C:18:LEU:O	1:C:82:LYS:HA	2.20	0.42
2:D:125:LEU:HD21	2:D:186:TYR:CD2	2.55	0.42
2:H:67:SER:HA	2:H:71:PHE:CE2	2.55	0.42
2:L:140:TYR:CG	2:L:141:PRO:HA	2.54	0.42
2:B:30:SER:O	2:B:71:PHE:CE2	2.73	0.41
1:C:126:VAL:HG22	1:C:147:VAL:HG13	2.00	0.41
1:E:51:TYR:CE2	1:E:59:ASP:HB3	2.55	0.41
2:F:50:TYR:O	2:F:52:SER:N	2.48	0.41
2:L:7:SER:HA	2:L:8:PRO:C	2.40	0.41
2:N:47:LEU:C	2:N:48:ILE:HD12	2.40	0.41
1:I:127:PHE:HE1	2:J:123:GLU:OE1	1.95	0.41
1:O:53:HIS:CE1	1:O:54:TYR:HE1	2.38	0.41
2:P:49:LYS:N	2:P:53:HIS:O	2.51	0.41
1:E:73:ASP:CG	1:E:76:LYS:HE2	2.41	0.41
1:E:88:ALA:C	1:E:90:ASP:H	2.23	0.41
1:G:127:PHE:HD2	1:G:146:LEU:HD23	1.85	0.41
1:G:154:PRO:O	1:G:205:HIS:HD2	2.03	0.41
2:L:90:GLN:NE2	2:L:97:THR:OG1	2.53	0.41
2:P:35:TRP:CE2	2:P:73:LEU:HB2	2.55	0.41
2:H:161:GLU:HA	2:H:176:SER:O	2.20	0.41
2:J:160:GLN:O	2:J:177:SER:HA	2.21	0.41
2:L:49:LYS:HB3	2:L:50:TYR:HD2	1.86	0.41
2:N:115:VAL:O	2:N:207:LYS:HD3	2.21	0.41
1:O:42:PRO:HD3	1:O:92:ALA:HA	2.02	0.41
1:A:189:VAL:HG21	1:A:194:LEU:HD21	2.01	0.41
1:G:144:GLY:HA3	1:G:186:VAL:HA	2.02	0.41
2:N:37:GLN:HG3	2:N:86:TYR:CE2	2.55	0.41
1:A:36:HIS:NE2	1:A:99:LYS:HD3	2.36	0.41
1:C:205:HIS:HB3	1:C:210:THR:HB	2.02	0.41
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.94	0.41
1:E:104:ALA:O	1:E:106:PRO:HD3	2.21	0.41
2:F:3:VAL:HG23	2:F:26:SER:HB3	2.03	0.41
1:G:71:SER:OG	3:G:318:HOH:O	2.10	0.41
1:K:176:GLN:HG3	1:K:180:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:ARG:HE	2:N:211:ARG:HB3	1.61	0.41
2:P:50:TYR:O	2:P:51:ALA:HB3	2.21	0.41
2:D:78:LEU:HD22	2:D:82:ASP:HB2	2.02	0.41
1:G:40:GLN:HB2	1:G:46:LEU:HD23	2.03	0.41
2:L:17:GLU:HG2	2:L:18:LYS:N	2.35	0.41
2:L:95:PRO:O	2:L:97:THR:HG23	2.21	0.41
2:L:122:ASP:O	2:L:126:LYS:HG2	2.21	0.41
1:M:14:PRO:O	1:M:15:SER:OG	2.33	0.41
1:M:95:TYR:CE2	2:N:43:SER:HB3	2.55	0.41
2:P:24:ARG:HG2	2:P:69:THR:HG22	2.02	0.41
2:B:190:LYS:O	2:B:210:ASN:HA	2.21	0.41
2:F:150:VAL:HG22	2:F:192:TYR:CD2	2.56	0.41
2:F:167:ASP:O	2:F:171:SER:HA	2.21	0.41
1:G:32:GLY:O	1:G:33:TYR:HB2	2.21	0.41
1:I:17:THR:HB	1:I:84:SER:HA	2.02	0.41
1:I:32:GLY:O	1:I:35:TRP:NE1	2.53	0.41
1:A:200:ILE:CD1	1:A:215:ARG:HD3	2.49	0.41
2:D:21:ILE:HD12	2:D:73:LEU:HD13	2.03	0.41
2:D:120:PRO:HD3	2:D:132:VAL:HG13	2.03	0.41
2:H:134:CYS:HB3	2:H:177:SER:OG	2.20	0.41
2:J:89:GLN:HG2	2:J:90:GLN:N	2.35	0.41
2:J:107:LYS:HD3	2:N:9:ASP:CG	2.41	0.41
1:K:48:TRP:HZ2	1:K:51:TYR:HD1	1.68	0.41
1:K:73:ASP:OD1	1:K:75:SER:OG	2.33	0.41
2:L:31:ASP:O	2:L:50:TYR:HA	2.20	0.41
2:L:139:PHE:CE1	2:L:174:SER:HA	2.55	0.41
1:M:69:THR:OG1	1:M:82:LYS:HB2	2.21	0.41
2:P:7:SER:OG	2:P:22:THR:OG1	2.38	0.41
2:B:34:HIS:O	2:B:88:CYS:HA	2.21	0.41
2:D:46:LEU:HD13	2:D:55:ILE:HD11	2.02	0.41
2:F:7:SER:HB3	2:L:17:GLU:OE1	2.21	0.41
1:G:161:SER:N	1:G:202:ASN:OD1	2.50	0.41
2:J:122:ASP:HA	2:J:125:LEU:HB2	2.03	0.41
1:K:14:PRO:HD2	1:K:118:SER:OG	2.21	0.41
2:N:89:GLN:HG3	2:N:98:PHE:CZ	2.55	0.41
1:O:104:ALA:O	1:O:106:PRO:HD3	2.21	0.41
1:C:39:ARG:O	1:C:47:GLU:N	2.50	0.40
2:D:125:LEU:HD23	2:D:183:LYS:HG3	2.03	0.40
2:D:139:PHE:HB2	2:D:198:HIS:CE1	2.56	0.40
2:J:33:LEU:HD13	2:J:34:HIS:N	2.36	0.40
2:J:50:TYR:N	2:J:51:ALA:CA	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:PHE:CD2	2:B:75:ILE:HG12	2.56	0.40
2:B:108:ARG:NH1	2:B:109:THR:HG23	2.36	0.40
2:F:186:TYR:CZ	2:F:211:ARG:HD3	2.57	0.40
2:J:13:VAL:HG22	2:N:8:PRO:HB3	2.02	0.40
2:N:3:VAL:HG12	3:N:320:HOH:O	2.21	0.40
2:P:13:VAL:CG1	2:P:17:GLU:HB3	2.51	0.40
2:P:145:LYS:HD2	2:P:197:THR:OG1	2.21	0.40
2:B:33:LEU:HD22	2:B:89:GLN:O	2.21	0.40
2:D:201:LEU:HD22	2:D:205:VAL:HG21	2.02	0.40
1:E:21:THR:HG23	1:E:80:SER:OG	2.22	0.40
2:H:167:ASP:OD1	2:H:169:LYS:N	2.49	0.40
1:I:164:LEU:HD23	1:I:164:LEU:HA	1.92	0.40
2:B:36:TYR:HE1	2:B:89:GLN:HB3	1.86	0.40
2:B:107:LYS:HA	2:B:140:TYR:OH	2.21	0.40
1:G:167:GLY:O	1:G:187:VAL:HA	2.22	0.40
2:H:140:TYR:CG	2:H:141:PRO:HA	2.56	0.40
1:K:200:ILE:CG2	1:K:213:ASP:HB3	2.52	0.40
2:N:50:TYR:O	2:N:51:ALA:HB3	2.21	0.40
2:P:15:PRO:O	2:P:16:LYS:HB2	2.21	0.40
1:A:190:PRO:O	1:A:193:SER:OG	2.39	0.40
1:C:115:THR:HG21	1:C:152:PRO:HB2	2.04	0.40
2:H:128:GLY:C	2:H:183:LYS:HB3	2.41	0.40
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.97	0.40
1:M:64:LEU:O	1:M:68:ILE:HG22	2.22	0.40
1:M:99:LYS:HG2	1:M:100:ASP:O	2.22	0.40
1:M:169:HIS:CE1	2:N:174:SER:HG	2.40	0.40
2:P:15:PRO:C	2:P:16:LYS:HD2	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:17:GLU:OE2	3:H:303:HOH:O[1_455]	2.01	0.19

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%)	205 (95%)	11 (5%)	0	100	100
1	C	206/225 (92%)	192 (93%)	13 (6%)	1 (0%)	29	47
1	E	205/225 (91%)	194 (95%)	10 (5%)	1 (0%)	29	47
1	G	184/225 (82%)	172 (94%)	12 (6%)	0	100	100
1	I	216/225 (96%)	203 (94%)	13 (6%)	0	100	100
1	K	195/225 (87%)	183 (94%)	12 (6%)	0	100	100
1	M	195/225 (87%)	185 (95%)	10 (5%)	0	100	100
1	O	205/225 (91%)	193 (94%)	12 (6%)	0	100	100
2	B	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	D	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
2	F	209/214 (98%)	194 (93%)	15 (7%)	0	100	100
2	H	210/214 (98%)	199 (95%)	11 (5%)	0	100	100
2	J	210/214 (98%)	198 (94%)	12 (6%)	0	100	100
2	L	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	29	47
2	N	209/214 (98%)	196 (94%)	13 (6%)	0	100	100
2	P	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
All	All	3296/3512 (94%)	3113 (94%)	180 (6%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	29	ILE
1	C	207	PRO
2	L	59	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	188/195 (96%)	165 (88%)	23 (12%)	5 7
1	C	182/195 (93%)	162 (89%)	20 (11%)	6 10
1	E	181/195 (93%)	153 (84%)	28 (16%)	2 3
1	G	163/195 (84%)	147 (90%)	16 (10%)	8 13
1	I	188/195 (96%)	159 (85%)	29 (15%)	2 3
1	K	174/195 (89%)	150 (86%)	24 (14%)	3 5
1	M	174/195 (89%)	148 (85%)	26 (15%)	3 4
1	O	181/195 (93%)	149 (82%)	32 (18%)	2 3
2	B	187/189 (99%)	154 (82%)	33 (18%)	2 3
2	D	186/189 (98%)	157 (84%)	29 (16%)	2 3
2	F	186/189 (98%)	151 (81%)	35 (19%)	1 2
2	H	187/189 (99%)	159 (85%)	28 (15%)	3 4
2	J	187/189 (99%)	162 (87%)	25 (13%)	4 5
2	L	187/189 (99%)	154 (82%)	33 (18%)	2 3
2	N	186/189 (98%)	158 (85%)	28 (15%)	3 4
2	P	186/189 (98%)	157 (84%)	29 (16%)	2 3
All	All	2923/3072 (95%)	2485 (85%)	438 (15%)	3 4

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLU
1	A	12	VAL
1	A	17	THR
1	A	18	LEU
1	A	19	SER
1	A	20	LEU
1	A	34	SER
1	A	44	LYS
1	A	65	LYS
1	A	67	ARG
1	A	69	THR
1	A	76	LYS
1	A	78	GLN
1	A	89	VAL
1	A	118	SER

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Mol	Chain	Res	Type
1	A	122	LYS
1	A	143	LEU
1	A	155	VAL
1	A	164	LEU
1	A	165	THR
1	A	193	SER
1	A	206	LYS
2	B	7	SER
2	B	12	SER
2	B	16	LYS
2	B	20	THR
2	B	23	CYS
2	B	27	GLN
2	B	28	SER
2	B	29	ILE
2	B	31	ASP
2	B	46	LEU
2	B	50	TYR
2	B	60	SER
2	B	73	LEU
2	B	76	ASN
2	B	77	SER
2	B	78	LEU
2	B	85	THR
2	B	90	GLN
2	B	108	ARG
2	B	109	THR
2	B	122	ASP
2	B	125	LEU
2	B	133	VAL
2	B	145	LYS
2	B	152	ASN
2	B	159	SER
2	B	176	SER
2	B	182	SER
2	B	183	LYS
2	B	185	ASP
2	B	187	GLU
2	B	194	CYS
2	B	203	SER
1	C	6	GLU
1	C	12	VAL

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Mol	Chain	Res	Type
1	C	17	THR
1	C	18	LEU
1	C	20	LEU
1	C	28	SER
1	C	65	LYS
1	C	71	SER
1	C	103	ASP
1	C	115	THR
1	C	118	SER
1	C	121	THR
1	C	125	SER
1	C	143	LEU
1	C	148	LYS
1	C	149	ASP
1	C	164	LEU
1	C	166	SER
1	C	187	VAL
1	C	206	LYS
2	D	3	VAL
2	D	12	SER
2	D	16	LYS
2	D	20	THR
2	D	26	SER
2	D	46	LEU
2	D	48	ILE
2	D	49	LYS
2	D	52	SER
2	D	56	SER
2	D	65	SER
2	D	73	LEU
2	D	74	THR
2	D	76	ASN
2	D	81	GLU
2	D	85	THR
2	D	88	CYS
2	D	90	GLN
2	D	96	LEU
2	D	129	THR
2	D	132	VAL
2	D	133	VAL
2	D	134	CYS
2	D	142	ARG

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Mol	Chain	Res	Type
2	D	161	GLU
2	D	183	LYS
2	D	195	GLU
2	D	201	LEU
2	D	210	ASN
1	E	4	LEU
1	E	6	GLU
1	E	13	LYS
1	E	17	THR
1	E	18	LEU
1	E	29	ILE
1	E	63	SER
1	E	66	THR
1	E	67	ARG
1	E	68	ILE
1	E	71	SER
1	E	74	THR
1	E	87	THR
1	E	96	CYS
1	E	115	THR
1	E	118	SER
1	E	120	SER
1	E	140	THR
1	E	164	LEU
1	E	176	GLN
1	E	184	SER
1	E	191	SER
1	E	192	SER
1	E	194	LEU
1	E	197	GLN
1	E	198	THR
1	E	209	ASN
1	E	214	LYS
2	F	7	SER
2	F	16	LYS
2	F	20	THR
2	F	28	SER
2	F	31	ASP
2	F	39	LYS
2	F	46	LEU
2	F	49	LYS
2	F	52	SER

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Mol	Chain	Res	Type
2	F	60	SER
2	F	73	LEU
2	F	74	THR
2	F	76	ASN
2	F	77	SER
2	F	78	LEU
2	F	79	GLU
2	F	81	GLU
2	F	85	THR
2	F	90	GLN
2	F	93	SER
2	F	96	LEU
2	F	109	THR
2	F	125	LEU
2	F	132	VAL
2	F	133	VAL
2	F	142	ARG
2	F	152	ASN
2	F	154	LEU
2	F	161	GLU
2	F	162	SER
2	F	164	THR
2	F	180	THR
2	F	183	LYS
2	F	203	SER
2	F	208	SER
1	G	1	GLN
1	G	6	GLU
1	G	12	VAL
1	G	17	THR
1	G	20	LEU
1	G	21	THR
1	G	67	ARG
1	G	71	SER
1	G	103	ASP
1	G	115	THR
1	G	121	THR
1	G	122	LYS
1	G	140	THR
1	G	156	THR
1	G	176	GLN
1	G	206	LYS

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Mol	Chain	Res	Type
2	H	14	THR
2	H	20	THR
2	H	22	THR
2	H	27	GLN
2	H	46	LEU
2	H	60	SER
2	H	73	LEU
2	H	74	THR
2	H	78	LEU
2	H	79	GLU
2	H	85	THR
2	H	90	GLN
2	H	97	THR
2	H	107	LYS
2	H	108	ARG
2	H	117	ILE
2	H	122	ASP
2	H	131	SER
2	H	154	LEU
2	H	155	GLN
2	H	156	SER
2	H	164	THR
2	H	169	LYS
2	H	183	LYS
2	H	185	ASP
2	H	188	LYS
2	H	203	SER
2	H	211	ARG
1	I	3	GLN
1	I	6	GLU
1	I	7	SER
1	I	12	VAL
1	I	13	LYS
1	I	14	PRO
1	I	15	SER
1	I	17	THR
1	I	20	LEU
1	I	21	THR
1	I	65	LYS
1	I	66	THR
1	I	69	THR
1	I	86	VAL

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Mol	Chain	Res	Type
1	I	103	ASP
1	I	110	GLN
1	I	118	SER
1	I	143	LEU
1	I	155	VAL
1	I	164	LEU
1	I	177	SER
1	I	184	SER
1	I	200	ILE
1	I	201	CYS
1	I	206	LYS
1	I	209	ASN
1	I	211	LYS
1	I	215	ARG
1	I	217	GLU
2	J	9	ASP
2	J	26	SER
2	J	30	SER
2	J	46	LEU
2	J	48	ILE
2	J	50	TYR
2	J	73	LEU
2	J	78	LEU
2	J	85	THR
2	J	90	GLN
2	J	96	LEU
2	J	103	LYS
2	J	108	ARG
2	J	125	LEU
2	J	126	LYS
2	J	142	ARG
2	J	154	LEU
2	J	164	THR
2	J	176	SER
2	J	180	THR
2	J	181	LEU
2	J	183	LYS
2	J	194	CYS
2	J	199	GLN
2	J	211	ARG
1	K	6	GLU
1	K	20	LEU

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Mol	Chain	Res	Type
1	K	21	THR
1	K	63	SER
1	K	64	LEU
1	K	65	LYS
1	K	67	ARG
1	K	76	LYS
1	K	86	VAL
1	K	89	VAL
1	K	96	CYS
1	K	100	ASP
1	K	115	THR
1	K	121	THR
1	K	122	LYS
1	K	125	SER
1	K	140	THR
1	K	166	SER
1	K	188	THR
1	K	209	ASN
1	K	211	LYS
1	K	213	ASP
1	K	214	LYS
1	K	215	ARG
2	L	14	THR
2	L	31	ASP
2	L	43	SER
2	L	46	LEU
2	L	48	ILE
2	L	60	SER
2	L	61	ARG
2	L	69	THR
2	L	73	LEU
2	L	77	SER
2	L	78	LEU
2	L	79	GLU
2	L	90	GLN
2	L	96	LEU
2	L	106	ILE
2	L	125	LEU
2	L	127	SER
2	L	129	THR
2	L	133	VAL
2	L	134	CYS

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Mol	Chain	Res	Type
2	L	154	LEU
2	L	159	SER
2	L	162	SER
2	L	164	THR
2	L	168	SER
2	L	177	SER
2	L	185	ASP
2	L	188	LYS
2	L	194	CYS
2	L	195	GLU
2	L	203	SER
2	L	208	SER
2	L	211	ARG
1	M	4	LEU
1	M	6	GLU
1	M	12	VAL
1	M	13	LYS
1	M	17	THR
1	M	18	LEU
1	M	20	LEU
1	M	34	SER
1	M	63	SER
1	M	66	THR
1	M	69	THR
1	M	84	SER
1	M	96	CYS
1	M	103	ASP
1	M	118	SER
1	M	125	SER
1	M	145	CYS
1	M	148	LYS
1	M	156	THR
1	M	164	LEU
1	M	188	THR
1	M	204	ASN
1	M	208	SER
1	M	209	ASN
1	M	210	THR
1	M	213	ASP
2	N	7	SER
2	N	18	LYS
2	N	20	THR

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Mol	Chain	Res	Type
2	N	26	SER
2	N	29	ILE
2	N	43	SER
2	N	46	LEU
2	N	50	TYR
2	N	56	SER
2	N	73	LEU
2	N	76	ASN
2	N	85	THR
2	N	88	CYS
2	N	90	GLN
2	N	105	GLU
2	N	107	LYS
2	N	125	LEU
2	N	126	LYS
2	N	142	ARG
2	N	164	THR
2	N	168	SER
2	N	180	THR
2	N	197	THR
2	N	199	GLN
2	N	203	SER
2	N	207	LYS
2	N	209	PHE
2	N	211	ARG
1	O	6	GLU
1	O	7	SER
1	O	17	THR
1	O	18	LEU
1	O	21	THR
1	O	44	LYS
1	O	52	ILE
1	O	54	TYR
1	O	64	LEU
1	O	66	THR
1	O	67	ARG
1	O	69	THR
1	O	71	SER
1	O	76	LYS
1	O	85	SER
1	O	86	VAL
1	O	99	LYS

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Mol	Chain	Res	Type
1	O	100	ASP
1	O	102	SER
1	O	110	GLN
1	O	112	THR
1	O	122	LYS
1	O	125	SER
1	O	148	LYS
1	O	156	THR
1	O	164	LEU
1	O	184	SER
1	O	191	SER
1	O	196	THR
1	O	211	LYS
1	O	214	LYS
1	O	217	GLU
2	P	5	THR
2	P	11	GLN
2	P	16	LYS
2	P	20	THR
2	P	29	ILE
2	P	31	ASP
2	P	46	LEU
2	P	49	LYS
2	P	73	LEU
2	P	78	LEU
2	P	85	THR
2	P	88	CYS
2	P	90	GLN
2	P	97	THR
2	P	108	ARG
2	P	109	THR
2	P	125	LEU
2	P	126	LYS
2	P	127	SER
2	P	129	THR
2	P	133	VAL
2	P	152	ASN
2	P	154	LEU
2	P	164	THR
2	P	180	THR
2	P	197	THR
2	P	199	GLN

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Mol	Chain	Res	Type
2	P	203	SER
2	P	210	ASN

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

Mol	Chain	Res	Type
2	B	124	GLN
2	D	147	GLN
1	E	169	HIS
2	F	11	GLN
2	F	53	HIS
2	F	137	ASN
1	G	3	GLN
2	H	11	GLN
2	H	90	GLN
2	H	124	GLN
1	I	1	GLN
1	I	3	GLN
1	I	5	GLN
2	J	32	HIS
2	J	90	GLN
1	M	204	ASN
2	N	90	GLN
2	N	92	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	0.09	5 (2%)	60	69	29, 42, 55, 64	0
1	C	210/225 (93%)	0.46	14 (6%)	17	21	38, 55, 84, 97	0
1	E	209/225 (92%)	0.63	19 (9%)	9	10	43, 58, 70, 80	0
1	G	190/225 (84%)	0.32	10 (5%)	26	31	28, 43, 70, 81	0
1	I	218/225 (96%)	0.20	8 (3%)	41	49	27, 42, 53, 68	0
1	K	201/225 (89%)	0.22	9 (4%)	33	39	30, 45, 62, 76	0
1	M	201/225 (89%)	0.45	15 (7%)	14	17	36, 54, 74, 85	0
1	O	209/225 (92%)	0.41	13 (6%)	20	25	41, 56, 68, 74	0
2	B	211/214 (98%)	0.14	2 (0%)	84	89	36, 49, 66, 78	0
2	D	211/214 (98%)	0.95	37 (17%)	1	1	36, 56, 75, 83	0
2	F	211/214 (98%)	0.53	19 (9%)	9	11	39, 52, 69, 79	0
2	H	212/214 (99%)	0.36	13 (6%)	21	26	32, 52, 78, 84	0
2	J	212/214 (99%)	0.23	5 (2%)	59	68	34, 48, 66, 72	0
2	L	211/214 (98%)	0.27	12 (5%)	23	28	32, 52, 74, 82	0
2	N	211/214 (98%)	0.50	17 (8%)	12	14	33, 54, 71, 81	0
2	P	211/214 (98%)	0.44	18 (8%)	10	13	35, 49, 67, 75	0
All	All	3346/3512 (95%)	0.39	216 (6%)	18	22	27, 51, 72, 97	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	205	VAL	6.9
1	I	42	PRO	6.7
1	M	213	ASP	6.7
2	L	128	GLY	6.5
2	D	118	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
2	D	202	SER	5.9
1	M	131	PRO	5.8
1	E	75	SER	5.8
2	L	123	GLU	5.5
2	F	202	SER	5.5
1	K	203	VAL	5.5
1	I	46	LEU	5.1
2	N	112	ALA	5.0
2	P	204	PRO	4.9
2	D	201	LEU	4.8
2	D	134	CYS	4.8
1	C	216	VAL	4.8
1	G	198	THR	4.7
1	M	170	THR	4.7
1	E	124	PRO	4.7
2	D	123	GLU	4.6
2	L	21	ILE	4.4
1	G	204	ASN	4.4
1	I	43	GLY	4.4
1	O	179	GLY	4.3
1	E	130	ALA	4.2
2	D	209	PHE	4.0
2	N	191	VAL	3.9
2	D	154	LEU	3.8
2	H	182	SER	3.8
1	C	129	LEU	3.8
1	M	129	LEU	3.7
2	J	67	SER	3.7
1	C	169	HIS	3.7
1	E	19	SER	3.7
2	D	116	PHE	3.7
1	O	131	PRO	3.7
1	E	216	VAL	3.6
2	N	161	GLU	3.6
2	P	149	LYS	3.6
2	N	162	SER	3.6
2	F	133	VAL	3.5
2	H	127	SER	3.5
2	D	67	SER	3.5
2	D	159	SER	3.5
1	M	171	PHE	3.4
1	M	130	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	191	VAL	3.4
2	H	128	GLY	3.4
1	C	170	THR	3.4
2	P	122	ASP	3.4
2	D	129	THR	3.3
2	J	75	ILE	3.3
1	E	154	PRO	3.3
2	F	142	ARG	3.2
2	H	122	ASP	3.2
1	C	157	VAL	3.2
1	E	65	LYS	3.2
2	P	210	ASN	3.2
2	P	189	HIS	3.2
1	G	129	LEU	3.2
2	D	157	GLY	3.2
2	F	157	GLY	3.1
2	F	67	SER	3.1
2	D	196	VAL	3.1
1	M	140	THR	3.1
1	C	4	LEU	3.0
2	D	130	ALA	3.0
1	O	187	VAL	3.0
1	I	1	GLN	3.0
1	C	84	SER	2.9
1	E	71	SER	2.9
2	D	207	LYS	2.9
2	N	192	TYR	2.9
1	O	42	PRO	2.9
2	N	148	TRP	2.9
2	P	67	SER	2.9
2	D	190	LYS	2.9
1	E	61	ASN	2.8
2	P	203	SER	2.8
1	E	79	PHE	2.8
2	P	135	LEU	2.8
2	P	134	CYS	2.8
1	O	120	SER	2.8
2	B	112	ALA	2.8
2	P	58	VAL	2.8
2	F	154	LEU	2.8
2	F	48	ILE	2.8
2	F	68	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	203	SER	2.8
2	H	183	LYS	2.8
2	D	186	TYR	2.7
2	D	70	ASP	2.7
2	D	192	TYR	2.7
2	D	189	HIS	2.7
2	N	189	HIS	2.7
2	F	118	PHE	2.7
1	M	1	GLN	2.7
1	M	212	VAL	2.7
1	K	110	GLN	2.7
1	O	172	PRO	2.6
1	G	126	VAL	2.6
1	I	209	ASN	2.6
1	M	61	ASN	2.6
1	G	164	LEU	2.6
1	I	10	GLY	2.6
1	M	218	PRO	2.6
1	M	65	LYS	2.6
1	O	105	PHE	2.6
1	I	87	THR	2.6
1	E	171	PHE	2.6
1	G	42	PRO	2.6
2	F	113	PRO	2.6
1	E	43	GLY	2.6
2	J	7	SER	2.6
2	F	190	LYS	2.5
2	N	205	VAL	2.5
1	G	178	SER	2.5
1	I	207	PRO	2.5
1	O	12	VAL	2.5
2	P	148	TRP	2.5
1	C	85	SER	2.5
2	D	160	GLN	2.5
2	L	67	SER	2.5
2	D	143	GLU	2.5
2	N	143	GLU	2.5
1	G	173	ALA	2.5
2	H	75	ILE	2.5
2	N	175	LEU	2.5
2	P	179	LEU	2.5
1	K	125	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	144	GLY	2.5
2	D	144	ALA	2.5
2	D	119	PRO	2.5
1	A	165	THR	2.5
1	E	103	ASP	2.5
2	H	21	ILE	2.5
2	P	211	ARG	2.5
2	H	123	GLU	2.4
2	H	126	LYS	2.4
2	D	75	ILE	2.4
1	E	182	SER	2.4
2	P	142	ARG	2.4
1	A	195	GLY	2.4
1	A	140	THR	2.4
1	G	120	SER	2.4
1	K	149	ASP	2.4
2	F	148	TRP	2.4
2	N	185	ASP	2.4
1	E	76	LYS	2.4
1	E	18	LEU	2.4
1	A	193	SER	2.4
2	D	178	THR	2.4
1	A	46	LEU	2.3
1	C	215	ARG	2.3
1	O	209	ASN	2.3
2	N	152	ASN	2.3
2	P	23	CYS	2.3
1	O	63	SER	2.3
2	F	104	VAL	2.3
1	K	213	ASP	2.3
2	J	202	SER	2.3
1	E	203	VAL	2.3
2	H	156	SER	2.3
2	L	126	LYS	2.3
1	C	213	ASP	2.3
2	J	21	ILE	2.3
2	H	73	LEU	2.2
1	E	206	LYS	2.2
2	D	146	VAL	2.2
1	O	177	SER	2.2
1	O	129	LEU	2.2
1	K	121	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	125	SER	2.2
2	F	35	TRP	2.2
2	D	206	THR	2.2
2	L	152	ASN	2.2
2	L	142	ARG	2.2
1	M	141	ALA	2.2
2	F	201	LEU	2.2
2	H	184	ALA	2.2
2	F	20	THR	2.2
2	H	72	THR	2.2
2	L	29	ILE	2.2
2	F	70	ASP	2.2
1	K	198	THR	2.2
2	L	127	SER	2.2
2	N	150	VAL	2.2
2	F	112	ALA	2.2
2	P	106	ILE	2.1
2	P	176	SER	2.1
2	D	2	ILE	2.1
2	N	3	VAL	2.1
2	P	195	GLU	2.1
2	F	205	VAL	2.1
1	K	215	ARG	2.1
1	M	46	LEU	2.1
1	C	65	LYS	2.1
2	D	127	SER	2.1
2	D	151	ASP	2.1
2	D	204	PRO	2.1
2	N	114	SER	2.1
2	D	136	LEU	2.1
1	G	201	CYS	2.1
2	B	121	SER	2.1
2	L	66	GLY	2.1
2	L	157	GLY	2.1
1	C	93	VAL	2.1
1	K	217	GLU	2.1
2	D	68	GLY	2.1
1	E	9	PRO	2.0
2	N	133	VAL	2.0
2	L	101	GLY	2.0
1	C	168	VAL	2.0
1	C	180	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	104	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.