Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 04:55 AM EDT

PDB ID	:	6OKQ
Title	:	Crystal structure of the SF12 Fab
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2019-04-14
Resolution	:	3.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

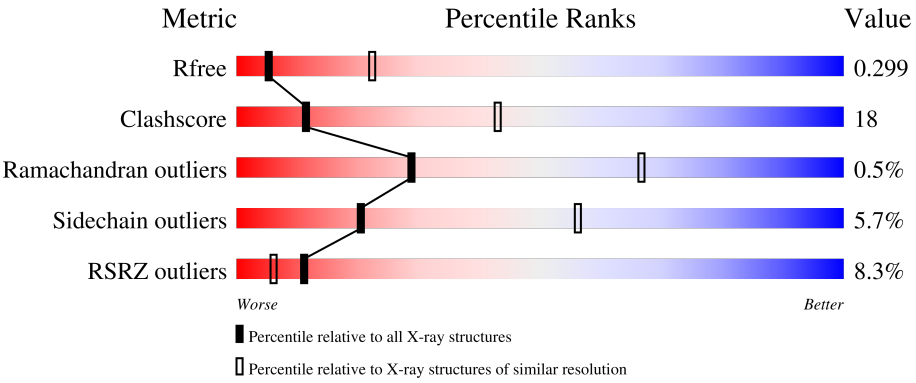
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	242	4% 61% 29% 5% • 5%
1	D	242	22% 65% 26% • • 5%
1	F	242	8% 59% 32% • 5%
2	B	211	68% 29% •
2	C	211	10% 69% 29% •

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Mol	Chain	Length	Quality of chain
2	E	211	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10056 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 SF12 Fab Heavy Chain,SF12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1735	1106	290	334	5			
1	D	230	Total	C	N	O	S	0	0	0
			1735	1106	290	334	5			
1	F	230	Total	C	N	O	S	0	0	0
			1735	1106	290	334	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	HIS	-	expression tag	UNP P0DOX5
A	222	HIS	-	expression tag	UNP P0DOX5
A	223	HIS	-	expression tag	UNP P0DOX5
A	224	HIS	-	expression tag	UNP P0DOX5
A	225	HIS	-	expression tag	UNP P0DOX5
D	221	HIS	-	expression tag	UNP P0DOX5
D	222	HIS	-	expression tag	UNP P0DOX5
D	223	HIS	-	expression tag	UNP P0DOX5
D	224	HIS	-	expression tag	UNP P0DOX5
D	225	HIS	-	expression tag	UNP P0DOX5
F	221	HIS	-	expression tag	UNP P0DOX5
F	222	HIS	-	expression tag	UNP P0DOX5
F	223	HIS	-	expression tag	UNP P0DOX5
F	224	HIS	-	expression tag	UNP P0DOX5
F	225	HIS	-	expression tag	UNP P0DOX5

- Molecule 2 is a protein called SF12 Fab Light Chain,SF12 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1617	1007	285	321	4			

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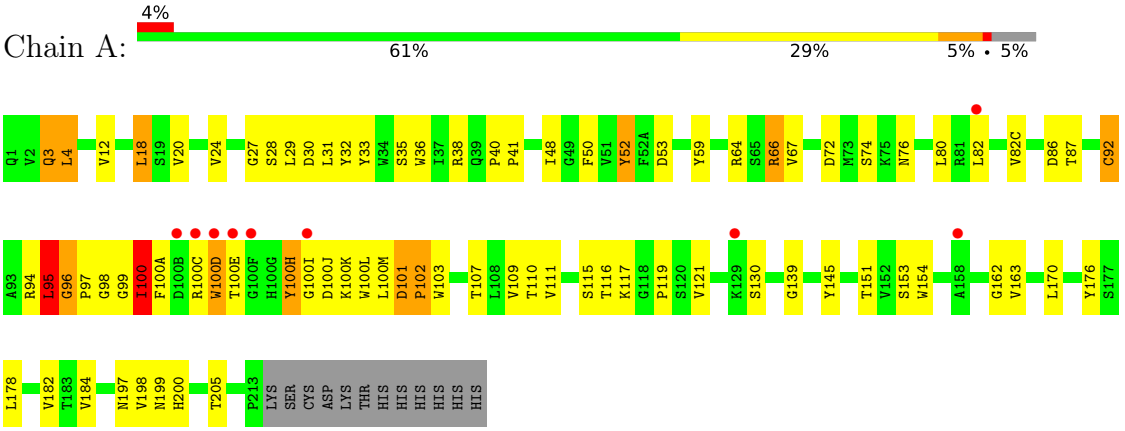
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1617	1007	285	321	4			
2	E	210	Total	C	N	O	S	0	0	0
			1617	1007	285	321	4			

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.

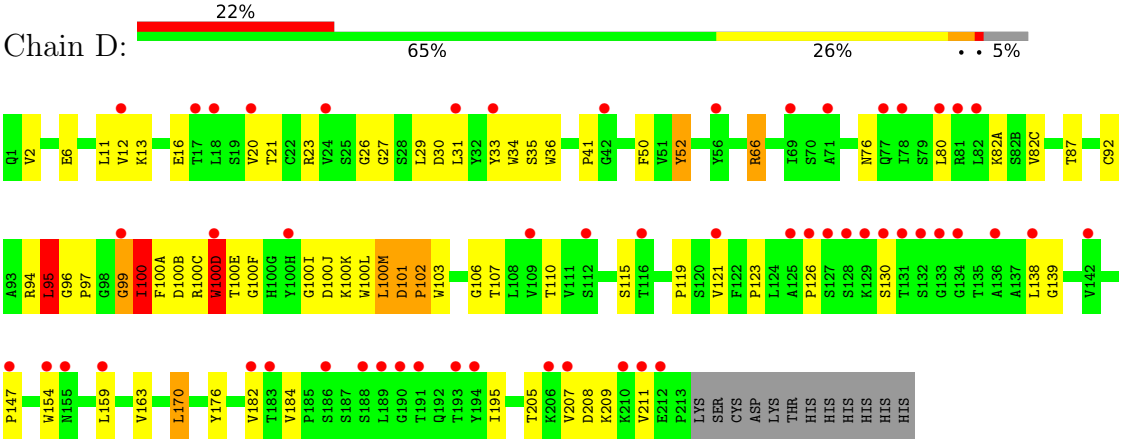
• Molecule 1: SF12 Fab Heavy Chain,SF12 Fab Heavy Chain

Chain A:



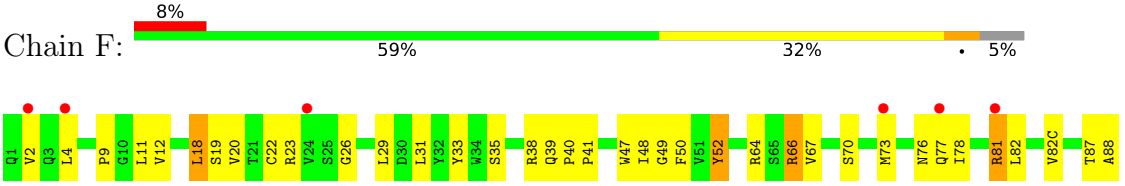
• Molecule 1: SF12 Fab Heavy Chain,SF12 Fab Heavy Chain

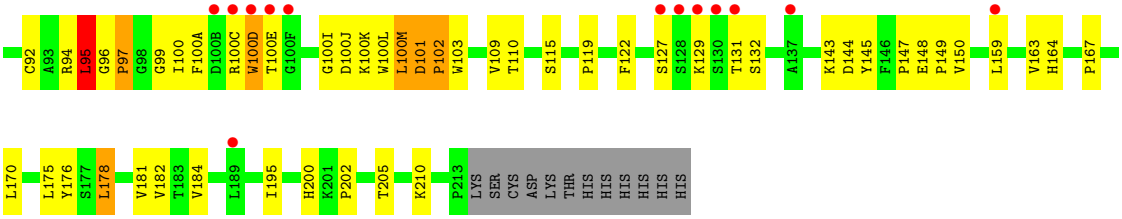
Chain D:



• Molecule 1: SF12 Fab Heavy Chain,SF12 Fab Heavy Chain

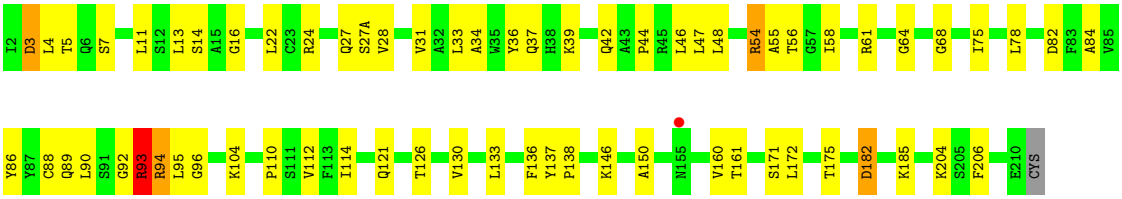
Chain F:





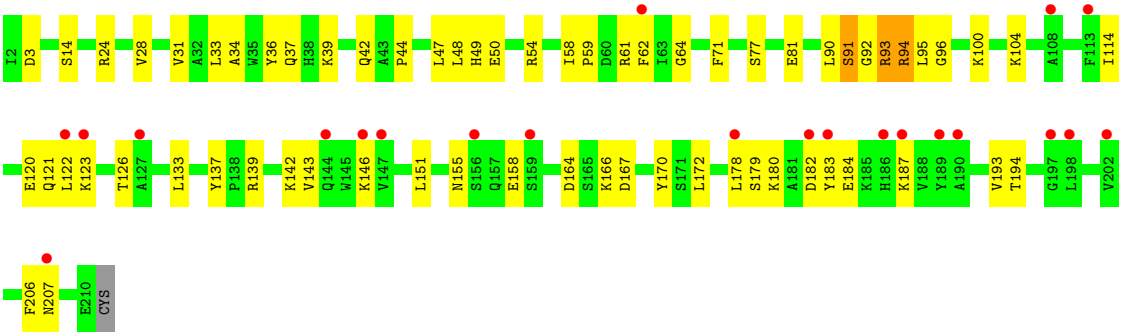
• Molecule 2: SF12 Fab Light Chain,SF12 Fab Light Chain

Chain B:



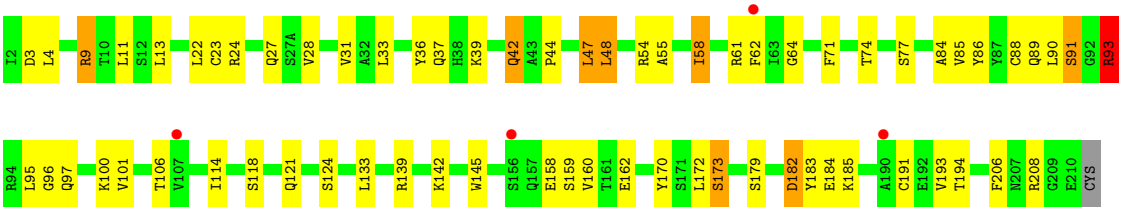
• Molecule 2: SF12 Fab Light Chain,SF12 Fab Light Chain

Chain C:



• Molecule 2: SF12 Fab Light Chain,SF12 Fab Light Chain

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	223.02Å 223.02Å 288.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.25 – 3.20 39.24 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.25-3.20) 99.9 (39.24-2.98)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.14_3219: ???)	Depositor
R, R_{free}	0.273 , 0.299 0.274 , 0.299	Depositor DCC
R_{free} test set	4344 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	94.8	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 127.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10056	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.60	0/1785	0.84	3/2440 (0.1%)
1	D	0.43	0/1785	0.68	2/2440 (0.1%)
1	F	0.48	1/1785 (0.1%)	0.73	1/2440 (0.0%)
2	B	0.56	0/1648	0.86	0/2235
2	C	0.43	0/1648	0.70	0/2235
2	E	0.55	0/1648	0.81	3/2235 (0.1%)
All	All	0.51	1/10299 (0.0%)	0.77	9/14025 (0.1%)

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	A	0	5
1	D	0	3
1	F	0	4
2	B	0	1
2	C	0	2
2	E	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	132	SER	CA-CB	5.83	1.61	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	48	LEU	CA-CB-CG	7.64	132.88	115.30
1	A	178	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	53	ASP	CB-CG-OD2	-5.39	113.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	170	LEU	CA-CB-CG	5.33	127.55	115.30
2	E	42	GLN	C-N-CA	-5.29	108.48	121.70
1	D	100(D)	TRP	CA-CB-CG	5.23	123.63	113.70
1	F	178	LEU	CA-CB-CG	5.19	127.23	115.30
2	E	47	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100(H)	TYR	Peptide
1	A	101	ASP	Peptide
1	A	95	LEU	Peptide
1	A	96	GLY	Peptide
1	A	99	GLY	Peptide
2	B	92	GLY	Peptide
2	C	92	GLY	Peptide
2	C	94	ARG	Peptide
1	D	101	ASP	Peptide
1	D	95	LEU	Peptide
1	D	99	GLY	Peptide
2	E	93	ARG	Peptide
1	F	101	ASP	Peptide
1	F	95	LEU	Peptide
1	F	97	PRO	Peptide
1	F	99	GLY	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	1735	0	1700	75	0
1	D	1735	0	1700	69	0
1	F	1735	0	1700	73	0
2	B	1617	0	1594	55	0
2	C	1617	0	1594	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1617	0	1594	56	0
All	All	10056	0	9882	353	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 18.

All (353) 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)
2:B:89:GLN:HG2	2:B:95:LEU:H	1.33	0.93
2:C:48:LEU:HD21	2:C:64:GLY:HA3	1.55	0.87
1:D:33:TYR:HB2	1:D:95:LEU:HB3	1.55	0.86
1:F:33:TYR:HB2	1:F:95:LEU:HB3	1.58	0.86
2:C:133:LEU:HB2	2:C:172:LEU:HB3	1.58	0.84
1:A:33:TYR:HB2	1:A:95:LEU:HB3	1.58	0.84
1:A:100(C):ARG:HG2	1:A:100(D):TRP:H	1.42	0.81
2:B:34:ALA:HB3	2:B:93:ARG:HH12	1.43	0.81
1:D:97:PRO:HD3	1:D:100(J):ASP:HA	1.63	0.81
2:B:54:ARG:HG2	2:B:58:ILE:HD11	1.63	0.81
1:A:100(K):LYS:HD2	2:B:31:VAL:HG12	1.63	0.80
2:E:48:LEU:HD21	2:E:64:GLY:HA3	1.64	0.80
1:A:35:SER:HB3	1:A:50:PHE:HB3	1.64	0.79
2:E:142:LYS:HB3	2:E:194:THR:HB	1.65	0.79
2:C:34:ALA:HB3	2:C:93:ARG:HH12	1.45	0.79
1:F:94:ARG:HH21	1:F:102:PRO:HD2	1.47	0.78
2:E:133:LEU:HD21	2:E:193:VAL:HG21	1.66	0.78
1:D:100(C):ARG:HG2	1:D:100(D):TRP:N	1.99	0.78
2:C:24:ARG:HB3	2:E:27:GLN:NE2	1.99	0.77
1:D:100(C):ARG:HD3	1:D:100(E):THR:HG23	1.66	0.75
1:A:18:LEU:HB3	1:A:82(C):VAL:HG21	1.68	0.75
2:E:133:LEU:HB2	2:E:172:LEU:HB3	1.69	0.74
2:C:133:LEU:HD21	2:C:193:VAL:HG21	1.70	0.74
1:D:96:GLY:HA2	1:D:100(L):TRP:H	1.53	0.73
1:D:87:THR:HG23	1:D:110:THR:HA	1.69	0.73
1:A:52:TYR:OH	1:A:100(A):PHE:HA	1.89	0.73
1:F:119:PRO:HD2	1:F:205:THR:HG21	1.69	0.73
2:B:54:ARG:HB2	2:B:54:ARG:HH11	1.54	0.73
2:E:93:ARG:HH21	2:E:93:ARG:HG3	1.52	0.72
1:F:96:GLY:HA2	1:F:100(K):LYS:H	1.53	0.72
2:B:36:TYR:OH	2:B:93:ARG:NH1	2.21	0.72
2:E:93:ARG:HH21	1:F:100(M):LEU:HD22	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:TYR:OH	1:F:100(A):PHE:HA	1.90	0.72
2:E:39:LYS:HB2	2:E:42:GLN:HG3	1.71	0.71
1:F:94:ARG:HB3	1:F:101:ASP:O	1.90	0.71
1:F:95:LEU:HD22	1:F:100(M):LEU:HD11	1.71	0.71
1:F:11:LEU:HD12	1:F:147:PRO:HG3	1.72	0.70
1:A:94:ARG:HB3	1:A:101:ASP:O	1.92	0.70
2:E:89:GLN:NE2	2:E:95:LEU:O	2.25	0.70
2:C:31:VAL:HG12	1:D:100(K):LYS:HD2	1.73	0.70
2:E:121:GLN:O	2:E:124:SER:OG	2.09	0.69
2:E:93:ARG:NH2	1:F:100(M):LEU:HD22	2.08	0.69
2:C:90:LEU:O	2:C:93:ARG:NH2	2.22	0.69
1:A:162:GLY:O	1:A:182:VAL:HA	1.93	0.69
1:D:100(C):ARG:HH11	1:D:100(E):THR:HG23	1.58	0.69
1:F:31:LEU:HD22	1:F:100(A):PHE:HB3	1.74	0.69
2:E:36:TYR:HE1	2:E:93:ARG:HH12	1.40	0.69
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.75	0.68
2:B:90:LEU:O	2:B:93:ARG:HD3	1.93	0.68
2:C:48:LEU:HD12	2:C:54:ARG:HA	1.75	0.68
1:A:94:ARG:HH21	1:A:102:PRO:HD2	1.59	0.68
1:A:100(C):ARG:HG2	1:A:100(D):TRP:N	2.07	0.68
2:C:114:ILE:HD12	2:C:206:PHE:HD2	1.58	0.67
1:F:100(C):ARG:HG2	1:F:100(D):TRP:H	1.59	0.67
1:A:18:LEU:HD12	1:A:109:VAL:HG11	1.77	0.67
1:A:100(E):THR:OG1	2:E:162:GLU:OE2	2.11	0.67
2:B:110:PRO:HB3	2:B:136:PHE:CD2	2.29	0.67
2:B:28:VAL:HG11	2:B:90:LEU:HD11	1.77	0.66
1:D:52:TYR:OH	1:D:100(A):PHE:HA	1.96	0.66
1:D:94:ARG:HH21	1:D:102:PRO:HD2	1.59	0.66
2:C:33:LEU:HG	2:C:34:ALA:N	2.12	0.65
2:E:58:ILE:HD11	2:E:62:PHE:HB2	1.79	0.65
2:E:95:LEU:HG	2:E:96:GLY:H	1.61	0.65
2:B:160:VAL:HB	2:B:172:LEU:HD12	1.78	0.65
1:F:97:PRO:HD3	1:F:100(J):ASP:HA	1.79	0.65
1:A:72:ASP:OD2	1:A:74:SER:OG	2.14	0.64
2:C:39:LYS:HB2	2:C:42:GLN:HG3	1.79	0.64
2:E:33:LEU:HD22	2:E:71:PHE:CD2	2.32	0.64
1:D:159:LEU:HD21	1:D:182:VAL:HG11	1.80	0.64
2:B:114:ILE:HD12	2:B:206:PHE:HD2	1.64	0.63
2:B:89:GLN:HG2	2:B:95:LEU:N	2.09	0.63
2:B:48:LEU:HD21	2:B:64:GLY:HA3	1.82	0.62
2:B:3:ASP:OD1	2:B:95:LEU:HD21	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:HA2	1:A:100(L):TRP:H	1.63	0.62
1:A:94:ARG:NH2	1:A:102:PRO:HD2	2.14	0.61
2:C:91:SER:O	2:C:93:ARG:HD3	1.99	0.61
1:A:18:LEU:HD23	1:A:82:LEU:HB3	1.82	0.61
1:F:2:VAL:HA	1:F:26:GLY:HA3	1.83	0.61
1:D:97:PRO:HD2	1:D:99:GLY:H	1.65	0.60
2:C:142:LYS:HB3	2:C:194:THR:HB	1.82	0.60
1:A:100(K):LYS:CD	2:B:31:VAL:HG12	2.30	0.60
2:E:44:PRO:HG2	1:F:103:TRP:CE3	2.36	0.60
1:F:97:PRO:HG3	1:F:100(I):GLY:CA	2.31	0.60
1:F:35:SER:HB3	1:F:50:PHE:HB3	1.84	0.60
1:A:32:TYR:HE1	1:A:94:ARG:NE	2.00	0.59
1:D:126:PRO:HD3	1:D:211:VAL:HG12	1.85	0.59
2:B:75:ILE:HG21	2:B:78:LEU:HD23	1.84	0.59
2:B:110:PRO:HB3	2:B:136:PHE:HD2	1.66	0.59
1:A:100(A):PHE:HZ	2:E:160:VAL:HB	1.67	0.59
2:B:39:LYS:HB2	2:B:42:GLN:HG3	1.85	0.59
2:C:44:PRO:HG2	1:D:103:TRP:CE3	2.37	0.59
1:A:97:PRO:HG3	1:A:100(J):ASP:N	2.18	0.58
2:B:133:LEU:HB2	2:B:172:LEU:HB3	1.83	0.58
2:B:48:LEU:CD2	2:B:64:GLY:HA3	2.33	0.58
1:A:31:LEU:HD22	1:A:100(A):PHE:HB3	1.85	0.58
1:A:97:PRO:HD3	1:A:100(J):ASP:HA	1.85	0.58
1:D:29:LEU:HA	1:D:34:TRP:CZ2	2.39	0.58
1:A:59:TYR:O	1:A:64:ARG:NH2	2.36	0.58
2:B:48:LEU:HD12	2:B:54:ARG:HA	1.84	0.58
1:A:153:SER:OG	1:A:197:ASN:HB2	2.03	0.58
1:A:121:VAL:HG21	1:A:198:VAL:HG21	1.84	0.58
1:F:18:LEU:HB3	1:F:82(C):VAL:HG21	1.84	0.58
2:B:14:SER:HA	2:B:104:LYS:O	2.04	0.57
1:A:82(C):VAL:HG12	1:A:111:VAL:HG11	1.85	0.57
2:E:9:ARG:NH2	2:E:97:GLN:O	2.38	0.57
1:A:4:LEU:HD13	1:A:92:CYS:SG	2.44	0.57
1:D:97:PRO:HD3	1:D:100(J):ASP:CA	2.34	0.57
2:B:54:ARG:HG2	2:B:58:ILE:CD1	2.33	0.57
2:C:28:VAL:HG11	2:C:90:LEU:HD11	1.87	0.57
1:A:36:TRP:CD1	1:A:80:LEU:HB2	2.39	0.57
1:A:87:THR:HG23	1:A:110:THR:HA	1.87	0.57
1:D:2:VAL:HA	1:D:26:GLY:HA3	1.87	0.57
2:E:184:GLU:HG2	2:E:208:ARG:NH1	2.20	0.56
1:F:94:ARG:NH2	1:F:102:PRO:HD2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:HIS:HD2	2:C:50:GLU:HG3	1.71	0.56
2:B:84:ALA:HB3	2:B:86:TYR:CE1	2.40	0.56
2:C:155:ASN:ND2	2:C:178:LEU:HD21	2.21	0.56
1:D:100(L):TRP:CZ3	1:D:101:ASP:HB2	2.41	0.56
1:F:87:THR:HG23	1:F:110:THR:HA	1.88	0.56
2:C:172:LEU:HD11	1:F:100(A):PHE:HZ	1.71	0.56
2:B:95:LEU:HG	2:B:96:GLY:H	1.70	0.56
1:A:103:TRP:CE3	2:B:44:PRO:HG2	2.40	0.55
1:F:96:GLY:CA	1:F:100(K):LYS:H	2.19	0.55
1:A:103:TRP:CD2	2:B:44:PRO:HG2	2.41	0.55
2:B:36:TYR:CE2	2:B:46:LEU:HD12	2.42	0.55
1:D:100(C):ARG:HG2	1:D:100(D):TRP:H	1.69	0.55
1:A:18:LEU:CD1	1:A:109:VAL:HG11	2.37	0.55
2:E:89:GLN:HB2	2:E:93:ARG:NH1	2.22	0.55
1:D:35:SER:HB3	1:D:50:PHE:HB3	1.88	0.55
2:E:39:LYS:HG2	2:E:84:ALA:HB2	1.89	0.55
1:A:12:VAL:HB	1:A:111:VAL:HG22	1.89	0.54
2:B:11:LEU:HD11	2:B:13:LEU:HD11	1.89	0.54
1:D:13:LYS:O	1:D:16:GLU:HB2	2.08	0.54
2:E:91:SER:O	2:E:93:ARG:HD2	2.07	0.54
1:D:31:LEU:O	1:D:99:GLY:HA3	2.07	0.54
1:F:100(C):ARG:HG2	1:F:100(D):TRP:N	2.21	0.54
1:A:100(A):PHE:CZ	2:E:160:VAL:HB	2.42	0.54
2:E:55:ALA:O	2:E:58:ILE:HG23	2.08	0.54
2:E:95:LEU:HG	2:E:96:GLY:N	2.23	0.54
2:B:182:ASP:O	2:B:185:LYS:HG2	2.08	0.54
1:F:95:LEU:HA	1:F:100(M):LEU:HD12	1.90	0.54
2:E:28:VAL:HG11	2:E:90:LEU:HD11	1.90	0.53
2:E:37:GLN:HG3	2:E:86:TYR:CE2	2.43	0.53
1:D:21:THR:HB	1:D:23:ARG:NH2	2.24	0.53
2:C:36:TYR:OH	2:C:93:ARG:NH1	2.42	0.53
1:D:66:ARG:HA	1:D:82(A):LYS:HD2	1.91	0.53
2:E:172:LEU:HG	2:E:173:SER:N	2.23	0.53
2:C:59:PRO:HG2	2:C:62:PHE:HE1	1.73	0.53
2:C:36:TYR:HH	1:D:100(M):LEU:H	1.55	0.53
1:D:163:VAL:HG22	1:D:182:VAL:HG22	1.90	0.53
1:D:97:PRO:HG3	1:D:100(I):GLY:CA	2.38	0.53
2:E:44:PRO:HG2	1:F:103:TRP:CD2	2.44	0.53
1:F:182:VAL:HG12	1:F:184:VAL:HG13	1.91	0.52
1:A:82(C):VAL:HG11	1:A:111:VAL:HG21	1.90	0.52
2:B:89:GLN:HG3	2:B:95:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:O	1:A:76:ASN:ND2	2.42	0.52
2:C:59:PRO:HG2	2:C:62:PHE:CE1	2.44	0.52
1:D:100(B):ASP:HB3	1:D:100(F):GLY:O	2.10	0.52
2:E:145:TRP:CZ3	2:E:191:CYS:HB2	2.45	0.52
2:C:81:GLU:HG2	2:C:166:LYS:NZ	2.25	0.51
2:E:159:SER:OG	1:F:167:PRO:HD2	2.10	0.51
2:B:94:ARG:CZ	2:B:95:LEU:HD22	2.41	0.51
1:A:100(L):TRP:CZ3	1:A:101:ASP:HB2	2.46	0.51
1:A:38:ARG:CB	1:A:48:ILE:HD11	2.41	0.51
2:C:122:LEU:HD21	2:C:183:TYR:CD2	2.46	0.51
2:C:180:LYS:NZ	2:C:184:GLU:OE2	2.40	0.50
1:D:100(C):ARG:NH1	1:D:100(E):THR:HG23	2.25	0.50
1:A:163:VAL:HG22	1:A:182:VAL:HG22	1.93	0.50
2:E:118:SER:OG	1:F:122:PHE:HB3	2.12	0.50
1:F:11:LEU:HD23	1:F:12:VAL:N	2.26	0.50
2:B:55:ALA:HB3	2:B:58:ILE:HG12	1.92	0.50
1:F:66:ARG:O	1:F:82:LEU:HD12	2.12	0.50
2:E:85:VAL:HG22	2:E:100:LYS:HA	1.92	0.50
1:F:159:LEU:HD21	1:F:182:VAL:HG11	1.94	0.50
1:F:96:GLY:N	1:F:100(L):TRP:O	2.40	0.50
2:B:7:SER:OG	2:B:22:LEU:HD23	2.11	0.50
2:B:121:GLN:HG2	2:B:126:THR:O	2.12	0.49
1:A:96:GLY:O	1:A:98:GLY:N	2.42	0.49
1:D:11:LEU:HD12	1:D:147:PRO:HG3	1.94	0.49
2:E:139:ARG:HB2	2:E:170:TYR:CE1	2.48	0.49
1:D:27:GLY:O	1:D:76:ASN:ND2	2.46	0.49
1:A:32:TYR:CE1	1:A:94:ARG:NE	2.81	0.49
1:F:95:LEU:HA	1:F:100(M):LEU:CD1	2.43	0.49
1:A:32:TYR:HE1	1:A:94:ARG:HE	1.58	0.48
1:A:130:SER:O	1:A:130:SER:OG	2.30	0.48
1:D:139:GLY:HA2	1:D:154:TRP:CH2	2.47	0.48
1:F:18:LEU:HD12	1:F:109:VAL:HG11	1.96	0.48
2:B:88:CYS:O	2:B:89:GLN:HG3	2.14	0.48
2:C:33:LEU:HD22	2:C:71:PHE:CD2	2.49	0.48
1:A:3:GLN:HG3	1:A:4:LEU:N	2.27	0.48
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.95	0.48
2:B:137:TYR:CG	2:B:138:PRO:HA	2.49	0.48
1:A:31:LEU:C	1:A:32:TYR:HD2	2.17	0.48
2:C:14:SER:HA	2:C:104:LYS:O	2.14	0.48
2:C:143:VAL:HG22	2:C:193:VAL:HG22	1.96	0.48
2:E:4:LEU:HD22	2:E:90:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:VAL:HG12	1:F:200:HIS:CD2	2.49	0.47
2:C:49:HIS:CD2	2:C:50:GLU:HG3	2.49	0.47
1:D:138:LEU:HB2	1:D:211:VAL:HG11	1.96	0.47
1:D:100(L):TRP:CE3	1:D:101:ASP:HB2	2.49	0.47
1:F:195:ILE:HD11	1:F:210:LYS:HE2	1.97	0.47
2:C:121:GLN:HG2	2:C:126:THR:O	2.15	0.47
2:E:93:ARG:HD3	1:F:100(M):LEU:HD13	1.95	0.47
1:A:66:ARG:O	1:A:82:LEU:HD12	2.14	0.47
2:B:4:LEU:HD12	2:B:4:LEU:HA	1.53	0.47
1:F:18:LEU:CB	1:F:82(C):VAL:HG21	2.45	0.47
1:F:163:VAL:HG22	1:F:182:VAL:HG22	1.97	0.47
1:A:28:SER:HA	1:A:76:ASN:HD21	1.79	0.47
1:A:52:TYR:HH	1:A:100(A):PHE:HA	1.79	0.47
2:B:27(A):SER:HA	2:B:68:GLY:O	2.15	0.47
1:F:143:LYS:HG2	1:F:144:ASP:OD2	2.15	0.47
1:A:38:ARG:HG2	1:A:40:PRO:HD3	1.97	0.47
1:F:97:PRO:HG3	1:F:100(I):GLY:HA3	1.96	0.47
1:F:100(M):LEU:HD12	1:F:100(M):LEU:HA	1.66	0.47
2:C:139:ARG:HB2	2:C:170:TYR:CE1	2.50	0.47
2:E:48:LEU:HD21	2:E:64:GLY:CA	2.41	0.47
1:D:96:GLY:N	1:D:100(L):TRP:O	2.48	0.46
1:D:36:TRP:CD1	1:D:80:LEU:HB2	2.49	0.46
1:F:144:ASP:HB3	1:F:175:LEU:HD13	1.97	0.46
1:D:6:GLU:CB	1:D:106:GLY:HA2	2.46	0.46
1:D:41:PRO:HB3	1:F:100(D):TRP:CE3	2.50	0.46
1:F:64:ARG:HA	1:F:67:VAL:HG12	1.96	0.46
1:D:119:PRO:HD2	1:D:205:THR:HG21	1.97	0.46
1:D:182:VAL:HG12	1:D:184:VAL:HG13	1.97	0.46
1:A:38:ARG:NH1	1:A:86:ASP:HA	2.31	0.46
2:E:47:LEU:HD22	2:E:58:ILE:HD13	1.97	0.46
1:D:95:LEU:HA	1:D:100(M):LEU:HD12	1.98	0.46
1:A:82(C):VAL:HG13	1:A:86:ASP:HB2	1.97	0.46
1:F:11:LEU:HD12	1:F:147:PRO:CG	2.41	0.46
2:C:93:ARG:HA	2:C:93:ARG:HD2	1.38	0.46
1:D:94:ARG:NH2	1:D:102:PRO:HD2	2.30	0.46
1:D:139:GLY:HA2	1:D:154:TRP:CZ2	2.51	0.45
1:A:100(M):LEU:HD23	1:A:103:TRP:CZ2	2.52	0.45
1:F:200:HIS:CG	1:F:202:PRO:HD2	2.50	0.45
2:E:183:TYR:CE1	2:E:208:ARG:HD3	2.50	0.45
1:F:38:ARG:HG2	1:F:40:PRO:HD3	1.99	0.45
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:ARG:HB2	1:F:48:ILE:HD11	1.98	0.45
1:F:148:GLU:OE2	1:F:149:PRO:HA	2.16	0.45
1:A:24:VAL:HG21	1:A:29:LEU:CD2	2.47	0.45
2:C:164:ASP:HB3	2:C:167:ASP:OD1	2.17	0.45
1:A:41:PRO:HD3	1:A:87:THR:O	2.17	0.45
2:C:95:LEU:HG	2:C:96:GLY:H	1.81	0.45
2:C:133:LEU:HD12	2:C:172:LEU:HD22	1.99	0.45
1:F:195:ILE:HG12	1:F:210:LYS:HG3	1.98	0.45
1:D:33:TYR:CE1	1:D:100(I):GLY:O	2.70	0.45
1:D:100(C):ARG:HH11	1:D:100(E):THR:CG2	2.29	0.44
1:D:170:LEU:HD13	1:D:176:TYR:CE1	2.52	0.44
2:E:61:ARG:HD2	2:E:77:SER:O	2.17	0.44
1:F:100(D):TRP:HD1	1:F:100(E):THR:N	2.16	0.44
1:A:97:PRO:HB3	1:A:100(K):LYS:HB2	2.00	0.44
1:F:100(D):TRP:CD1	1:F:100(E):THR:N	2.85	0.44
1:A:145:TYR:CE1	1:A:176:TYR:HB2	2.52	0.44
2:B:28:VAL:HG11	2:B:90:LEU:CD1	2.46	0.44
2:C:133:LEU:HD21	2:C:193:VAL:CG2	2.43	0.44
2:B:33:LEU:HG	2:B:34:ALA:N	2.31	0.44
1:F:81:ARG:CZ	1:F:81:ARG:HB3	2.47	0.44
1:D:130:SER:O	1:D:130:SER:OG	2.35	0.44
2:C:44:PRO:HG2	1:D:103:TRP:CD2	2.53	0.44
1:D:95:LEU:HD22	1:D:100(M):LEU:HD11	2.00	0.44
1:D:100:ILE:H	1:D:100:ILE:HG13	1.43	0.44
1:D:170:LEU:HD13	1:D:176:TYR:CZ	2.52	0.44
2:B:112:VAL:HG12	2:B:204:LYS:HD2	1.99	0.44
1:D:66:ARG:H	1:D:66:ARG:HG3	1.67	0.44
1:A:95:LEU:HD22	1:A:100(M):LEU:HD11	2.00	0.43
2:C:122:LEU:O	2:C:180:LYS:HD2	2.18	0.43
1:D:123:PRO:HD3	1:D:209:LYS:HG2	2.00	0.43
2:B:61:ARG:HH21	2:B:82:ASP:CG	2.20	0.43
2:B:94:ARG:HE	2:B:94:ARG:HB2	1.28	0.43
1:F:29:LEU:HD12	1:F:73:MET:HA	2.01	0.43
2:B:5:THR:O	2:B:24:ARG:N	2.42	0.43
1:A:82(C):VAL:CG1	1:A:111:VAL:HG21	2.48	0.43
2:B:39:LYS:HG2	2:B:84:ALA:HB2	2.00	0.43
1:D:41:PRO:HD3	1:D:87:THR:O	2.18	0.43
2:E:179:SER:OG	2:E:182:ASP:HB2	2.19	0.43
1:A:94:ARG:NH2	1:A:101:ASP:HB3	2.33	0.43
1:D:100(C):ARG:CD	1:D:100(E):THR:HG23	2.44	0.43
1:D:121:VAL:O	1:D:209:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:PRO:HD3	1:F:87:THR:O	2.19	0.43
2:C:104:LYS:HA	2:C:137:TYR:OH	2.19	0.43
2:B:16:GLY:N	2:B:78:LEU:O	2.51	0.43
2:C:61:ARG:HD2	2:C:77:SER:O	2.18	0.43
2:C:24:ARG:HD3	2:E:27:GLN:HE21	1.83	0.43
2:C:54:ARG:HG2	2:C:58:ILE:HD11	2.01	0.43
2:C:146:LYS:HG2	2:C:151:LEU:HD23	2.01	0.43
1:F:127:SER:O	1:F:131:THR:HG23	2.18	0.43
1:F:170:LEU:HD13	1:F:176:TYR:CD2	2.53	0.43
1:A:151:THR:HB	1:A:199:ASN:HB3	2.00	0.43
2:C:31:VAL:HG12	1:D:100(K):LYS:CD	2.44	0.43
2:E:4:LEU:HD12	2:E:4:LEU:HA	1.82	0.43
1:D:97:PRO:CD	1:D:99:GLY:H	2.28	0.42
2:E:88:CYS:O	2:E:89:GLN:HG3	2.19	0.42
2:B:58:ILE:H	2:B:58:ILE:HG13	1.69	0.42
1:F:150:VAL:HG12	1:F:200:HIS:HD2	1.83	0.42
2:C:36:TYR:OH	1:D:100(M):LEU:HB2	2.20	0.42
1:F:22:CYS:O	1:F:77:GLN:HA	2.20	0.42
2:B:130:VAL:HG22	2:B:175:THR:OG1	2.19	0.42
1:F:35:SER:HA	1:F:50:PHE:HA	2.02	0.42
1:F:97:PRO:HD3	1:F:100(J):ASP:CA	2.48	0.42
1:A:18:LEU:CD2	1:A:82:LEU:HB3	2.49	0.42
1:A:97:PRO:HG3	1:A:100(I):GLY:CA	2.50	0.42
2:B:146:LYS:HA	2:B:150:ALA:O	2.19	0.42
2:B:36:TYR:CD2	2:B:46:LEU:HA	2.55	0.41
1:A:100(H):TYR:CD2	2:E:100:LYS:HD3	2.54	0.41
2:B:27:GLN:HG2	2:E:24:ARG:HD3	2.01	0.41
2:B:161:THR:HG23	2:B:171:SER:O	2.20	0.41
2:C:126:THR:HA	2:C:179:SER:HA	2.01	0.41
2:E:93:ARG:HG3	2:E:93:ARG:NH2	2.29	0.41
1:D:209:LYS:HB2	1:D:209:LYS:HE2	1.83	0.41
1:A:119:PRO:HD2	1:A:205:THR:HG21	2.01	0.41
2:B:137:TYR:CD1	2:B:138:PRO:HA	2.56	0.41
2:C:94:ARG:HH21	2:C:95:LEU:HD13	1.86	0.41
1:D:195:ILE:CG2	1:D:208:ASP:HB3	2.51	0.41
2:E:48:LEU:HD12	2:E:54:ARG:HA	2.01	0.41
1:F:47:TRP:CZ2	1:F:49:GLY:HA2	2.54	0.41
1:D:100(M):LEU:HD23	1:D:103:TRP:CZ2	2.55	0.41
1:D:154:TRP:HB3	1:D:159:LEU:HB3	2.02	0.41
1:D:154:TRP:CE2	1:D:182:VAL:HG23	2.56	0.41
1:F:9:PRO:HD2	1:F:19:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:TYR:CE1	1:F:150:VAL:HG13	2.56	0.41
1:F:164:HIS:HB2	1:F:181:VAL:HG23	2.02	0.41
1:A:100(C):ARG:HG3	1:F:167:PRO:HB3	2.01	0.41
1:A:100(J):ASP:N	1:A:100(J):ASP:OD1	2.54	0.41
1:A:182:VAL:HG12	1:A:184:VAL:HG13	2.02	0.41
2:E:28:VAL:HG11	2:E:90:LEU:CD1	2.50	0.41
1:F:70:SER:O	1:F:78:ILE:HG23	2.19	0.41
2:E:89:GLN:HG2	2:E:95:LEU:H	1.85	0.41
2:C:94:ARG:HG3	2:C:95:LEU:HB2	2.03	0.41
2:C:122:LEU:HD22	2:C:180:LYS:HG3	2.03	0.41
2:C:187:LYS:HB3	2:C:207:ASN:OD1	2.21	0.41
1:D:11:LEU:HD12	1:D:147:PRO:HD3	2.03	0.41
1:F:39:GLN:O	1:F:88:ALA:HB1	2.21	0.41
1:A:100:ILE:H	1:A:100:ILE:HG13	1.32	0.41
1:D:100(C):ARG:HE	1:D:100(D):TRP:HD1	1.68	0.41
2:E:31:VAL:HG12	1:F:100(K):LYS:CD	2.51	0.41
1:F:170:LEU:HD13	1:F:176:TYR:CE2	2.56	0.41
1:A:95:LEU:HD12	1:A:96:GLY:HA3	2.03	0.40
1:A:139:GLY:HA2	1:A:154:TRP:CZ2	2.56	0.40
2:E:11:LEU:HD11	2:E:13:LEU:HD11	2.03	0.40
2:E:22:LEU:HD12	2:E:23:CYS:N	2.36	0.40
1:A:97:PRO:HG3	1:A:100(I):GLY:C	2.41	0.40
1:F:150:VAL:HG22	1:F:178:LEU:HD13	2.03	0.40
1:A:170:LEU:HD13	1:A:176:TYR:CE1	2.57	0.40
1:D:100(K):LYS:HB2	1:D:100(K):LYS:HE2	1.79	0.40
2:E:11:LEU:O	2:E:101:VAL:HA	2.21	0.40
2:C:122:LEU:HD22	2:C:180:LYS:HE2	2.04	0.40
2:C:126:THR:HG23	2:C:178:LEU:O	2.21	0.40
1:A:67:VAL:HG23	1:A:82:LEU:HD13	2.03	0.40
1:A:117:LYS:O	1:A:200:HIS:HE1	2.04	0.40
2:C:120:GLU:HA	2:C:123:LYS:HD2	2.02	0.40
1:D:11:LEU:HD23	1:D:12:VAL:N	2.37	0.40
1:D:100(M):LEU:HD12	1:D:100(M):LEU:HA	1.70	0.40
2:E:206:PHE:HB3	1:F:129:LYS:HG3	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	228/242 (94%)	206 (90%)	20 (9%)	2 (1%)	17 56
1	D	228/242 (94%)	209 (92%)	17 (8%)	2 (1%)	17 56
1	F	228/242 (94%)	211 (92%)	15 (7%)	2 (1%)	17 56
2	B	208/211 (99%)	193 (93%)	14 (7%)	1 (0%)	29 67
2	C	208/211 (99%)	195 (94%)	13 (6%)	0	100 100
2	E	208/211 (99%)	189 (91%)	19 (9%)	0	100 100
All	All	1308/1359 (96%)	1203 (92%)	98 (8%)	7 (0%)	29 67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	D	100	ILE
1	A	102	PRO
1	F	102	PRO
1	D	102	PRO
1	F	100	ILE
2	B	93	ARG

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	195/208 (94%)	181 (93%)	14 (7%)	14 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	195/208 (94%)	182 (93%)	13 (7%)	16 50
1	F	195/208 (94%)	182 (93%)	13 (7%)	16 50
2	B	181/182 (100%)	175 (97%)	6 (3%)	38 71
2	C	181/182 (100%)	175 (97%)	6 (3%)	38 71
2	E	181/182 (100%)	169 (93%)	12 (7%)	16 51
All	All	1128/1170 (96%)	1064 (94%)	64 (6%)	20 56

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	LEU
1	A	18	LEU
1	A	20	VAL
1	A	30	ASP
1	A	52	TYR
1	A	66	ARG
1	A	92	CYS
1	A	95	LEU
1	A	100	ILE
1	A	100(D)	TRP
1	A	107	THR
1	A	115	SER
1	A	116	THR
2	B	3	ASP
2	B	54	ARG
2	B	56	THR
2	B	93	ARG
2	B	94	ARG
2	B	182	ASP
2	C	3	ASP
2	C	91	SER
2	C	93	ARG
2	C	100	LYS
2	C	158	GLU
2	C	182	ASP
1	D	20	VAL
1	D	30	ASP
1	D	52	TYR
1	D	66	ARG

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Mol	Chain	Res	Type
1	D	82(C)	VAL
1	D	92	CYS
1	D	95	LEU
1	D	100	ILE
1	D	100(D)	TRP
1	D	100(M)	LEU
1	D	107	THR
1	D	115	SER
1	D	207	VAL
2	E	3	ASP
2	E	9	ARG
2	E	58	ILE
2	E	74	THR
2	E	91	SER
2	E	93	ARG
2	E	106	THR
2	E	114	ILE
2	E	158	GLU
2	E	173	SER
2	E	182	ASP
2	E	185	LYS
1	F	4	LEU
1	F	18	LEU
1	F	20	VAL
1	F	23	ARG
1	F	52	TYR
1	F	66	ARG
1	F	76	ASN
1	F	81	ARG
1	F	92	CYS
1	F	95	LEU
1	F	100(D)	TRP
1	F	100(M)	LEU
1	F	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	49	HIS
2	E	27	GLN
2	E	186	HIS

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 monosaccharides 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	230/242 (95%)	0.20	9 (3%) 39 25	108, 132, 166, 198	0
1	D	230/242 (95%)	1.20	54 (23%) 0 0	170, 200, 230, 237	0
1	F	230/242 (95%)	0.48	19 (8%) 11 6	132, 164, 192, 208	0
2	B	210/211 (99%)	0.01	1 (0%) 91 86	108, 128, 147, 175	0
2	C	210/211 (99%)	0.55	22 (10%) 6 3	138, 183, 224, 233	0
2	E	210/211 (99%)	0.14	4 (1%) 66 53	118, 150, 166, 189	0
All	All	1320/1359 (97%)	0.44	109 (8%) 11 6	108, 155, 221, 237	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	TYR	10.4
1	F	130	SER	8.7
2	C	189	TYR	8.4
1	F	129	LYS	7.5
1	D	193	THR	6.4
1	D	127	SER	6.3
2	C	146	LYS	6.3
2	C	190	ALA	6.2
1	D	129	LYS	5.7
1	D	130	SER	5.6
1	D	126	PRO	5.5
2	C	197	GLY	5.3
1	D	18	LEU	4.9
1	D	159	LEU	4.8
2	C	202	VAL	4.5
1	D	189	LEU	4.3
1	D	131	THR	4.2
1	D	207	VAL	4.1
2	C	113	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	128	SER	3.9
2	C	122	LEU	3.8
2	C	127	ALA	3.8
1	F	2	VAL	3.8
1	A	129	LYS	3.7
1	D	69	ILE	3.6
1	D	142	VAL	3.5
1	D	191	THR	3.5
2	C	159	SER	3.3
2	C	186	HIS	3.3
1	D	190	GLY	3.3
1	A	100(F)	GLY	3.3
1	D	210	LYS	3.3
1	F	100(E)	THR	3.3
1	D	77	GLN	3.2
1	D	211	VAL	3.2
1	D	147	PRO	3.2
1	D	182	VAL	3.0
1	F	159	LEU	3.0
1	D	138	LEU	3.0
1	D	31	LEU	3.0
1	D	82	LEU	2.9
1	D	132	SER	2.9
1	A	100(C)	ARG	2.9
2	C	207	ASN	2.8
1	A	82	LEU	2.8
2	C	183	TYR	2.8
1	A	100(E)	THR	2.8
1	D	17	THR	2.8
1	F	4	LEU	2.8
1	D	136	ALA	2.7
1	D	134	GLY	2.7
1	D	121	VAL	2.7
1	F	81	ARG	2.7
1	F	128	SER	2.7
1	F	131	THR	2.7
1	F	100(F)	GLY	2.7
1	D	100(D)	TRP	2.6
1	D	12	VAL	2.6
1	D	33	TYR	2.6
1	D	71	ALA	2.6
1	D	100(H)	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	81	ARG	2.5
2	E	190	ALA	2.5
2	C	182	ASP	2.5
1	D	206	LYS	2.5
1	F	100(B)	ASP	2.5
2	C	198	LEU	2.5
1	D	183	THR	2.5
1	D	109	VAL	2.4
1	D	154	TRP	2.4
2	C	62	PHE	2.4
2	E	62	PHE	2.4
1	D	56	TYR	2.4
2	C	108	ALA	2.4
2	C	187	LYS	2.4
1	D	212	GLU	2.4
1	F	137	ALA	2.4
2	C	144	GLN	2.3
1	D	20	VAL	2.3
1	D	133	GLY	2.3
1	A	100(B)	ASP	2.3
2	E	107	VAL	2.3
1	D	42	GLY	2.3
1	D	99	GLY	2.3
1	D	80	LEU	2.3
2	C	178	LEU	2.3
2	B	155	ASN	2.3
1	D	116	THR	2.3
2	C	147	VAL	2.2
1	D	188	SER	2.2
1	F	24	VAL	2.2
1	F	73	MET	2.2
1	D	112	SER	2.2
1	F	189	LEU	2.2
1	D	78	ILE	2.2
1	F	127	SER	2.1
1	D	125	ALA	2.1
1	F	100(D)	TRP	2.1
2	C	156	SER	2.1
1	D	155	ASN	2.1
1	A	158	ALA	2.1
1	A	100(D)	TRP	2.1
1	A	100(I)	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	77	GLN	2.1
1	D	186	SER	2.1
2	E	156	SER	2.1
1	D	24	VAL	2.0
1	F	100(C)	ARG	2.0
2	C	123	LYS	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.