Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 03:02 AM JST

PDB ID	:	8GV0
Title	:	Crystal structure of anti-FIXa IgG fab without FAST-Ig mutations
Authors	:	Koga, H.; Yamano, T.; Fukami, T.A.; Sampei, Z.; Shiraiwa, H.; Torizawa, T.
Deposited on	:	2022-09-14
Resolution	:	3.19 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:

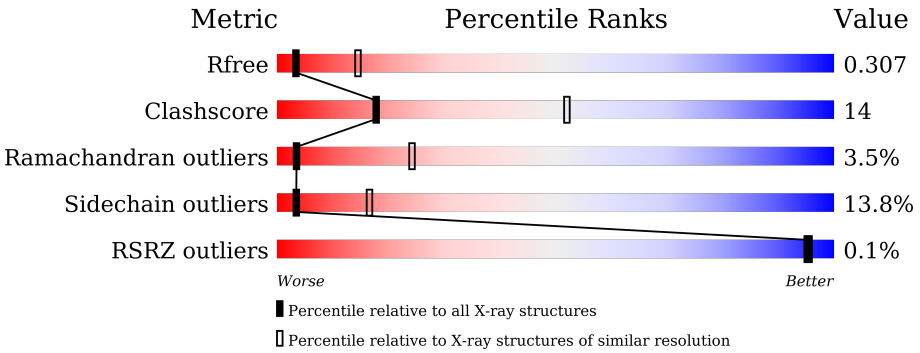
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.19 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	227	70% 23%
1	C	227	64% 29% 5%
1	E	227	63% 30% 5%
1	G	227	74% 18%
2	B	214	62% 35%
2	D	214	59% 35% 6%

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Mol	Chain	Length	Quality of chain
2	F	214	
2	H	214	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12316 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 Anti-factor IXa IgG fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1596	1009	267	314	6			
1	C	223	Total	C	N	O	S	0	0	0
			1576	985	264	322	5			
1	E	216	Total	C	N	O	S	0	0	0
			1533	963	257	308	5			
1	G	220	Total	C	N	O	S	0	0	0
			1477	923	243	306	5			

- Molecule 2 is a protein called Anti-factor IXa IgG fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1551	966	259	321	5			
2	D	214	Total	C	N	O	S	0	0	0
			1535	958	255	317	5			
2	F	214	Total	C	N	O	S	0	0	0
			1547	958	263	321	5			
2	H	214	Total	C	N	O	S	0	0	0
			1461	910	239	307	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	4	Total	O	0	0
			4	4		
3	C	4	Total	O	0	0
			4	4		
3	D	6	Total	O	0	0
			6	6		

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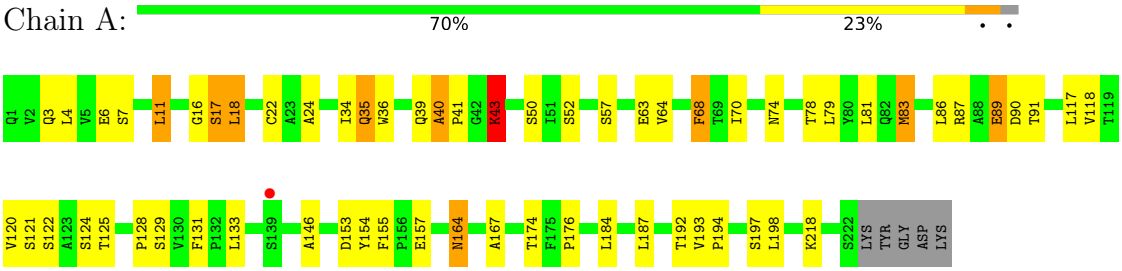
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total O 2 2	0	0
3	F	10	Total O 10 10	0	0
3	G	2	Total O 2 2	0	0
3	H	5	Total O 5 5	0	0

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.

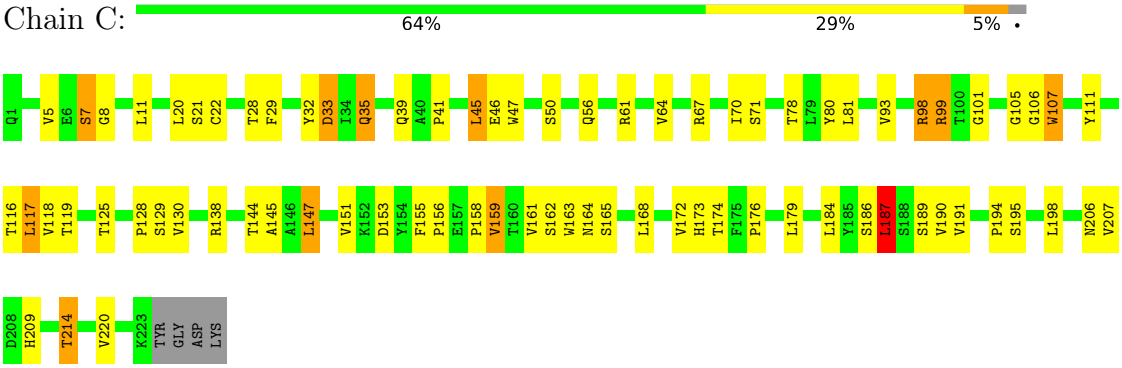
• Molecule 1: Anti-factor IXa IgG fab heavy chain

Chain A:



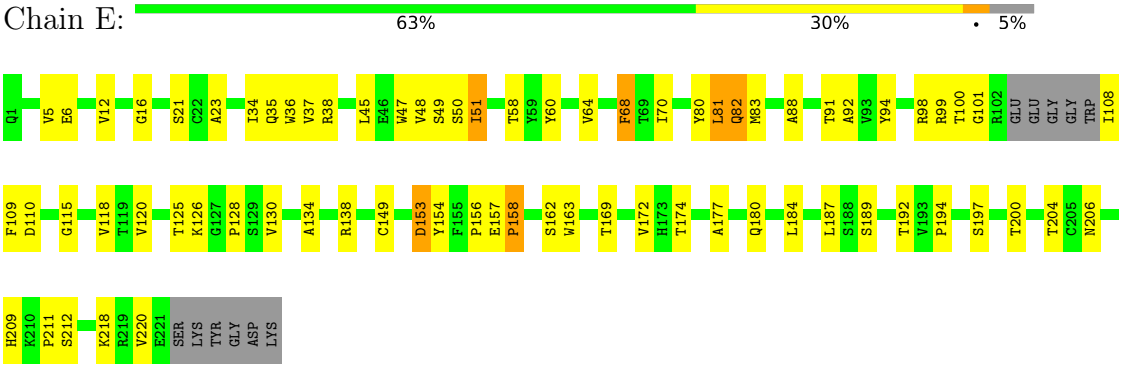
• Molecule 1: Anti-factor IXa IgG fab heavy chain

Chain C:



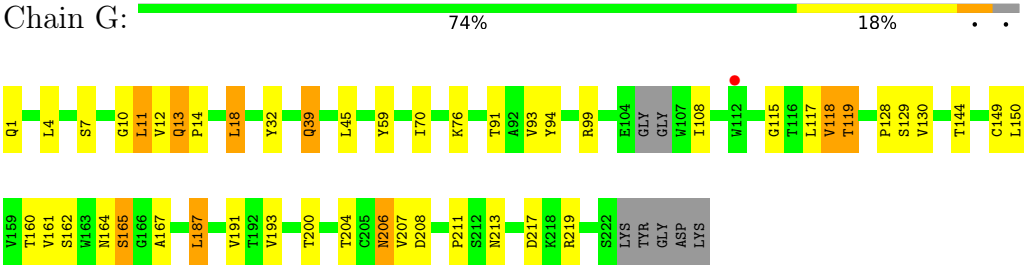
• Molecule 1: Anti-factor IXa IgG fab heavy chain

Chain E:



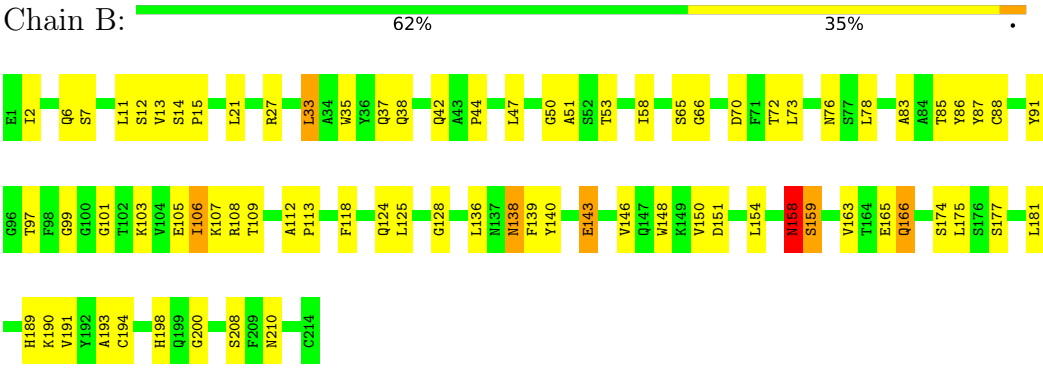
• Molecule 1: Anti-factor IXa IgG fab heavy chain

Chain G:



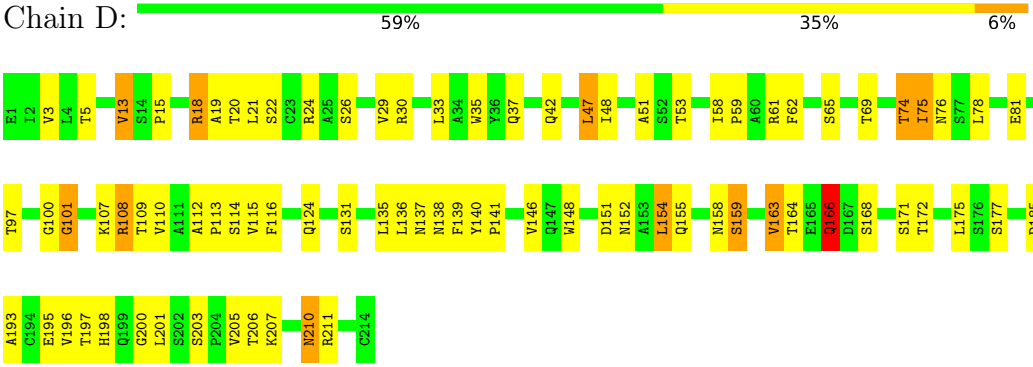
• Molecule 2: Anti-factor IXa IgG fab light chain

Chain B:



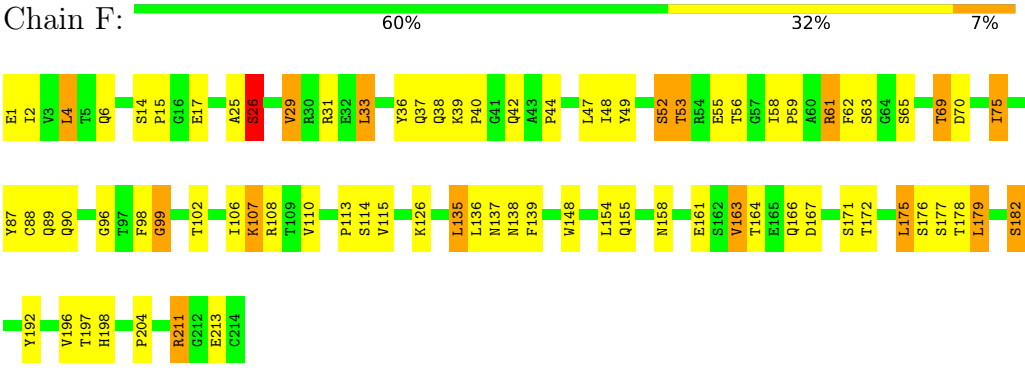
• Molecule 2: Anti-factor IXa IgG fab light chain

Chain D:



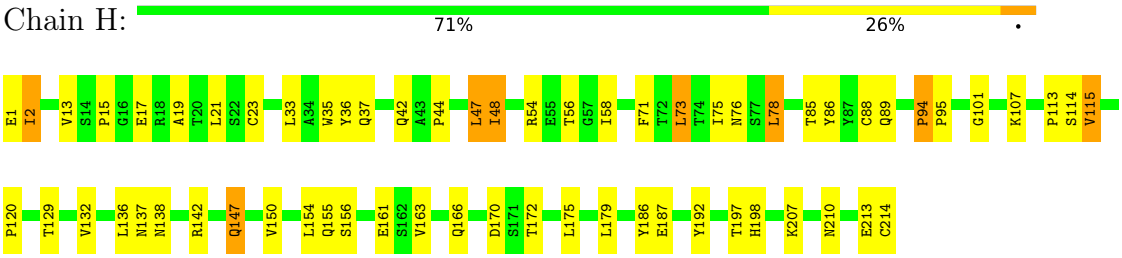
• Molecule 2: Anti-factor IXa IgG fab light chain

Chain F:



• Molecule 2: Anti-factor IXa IgG fab light chain

Chain H:


71%
26%
E1 I2 V13 S14 P15 G16 E17 R18 A19 T20 L21 S22 C23 L33 A34 W35 Y36 Q37 Q42 A43 P44 L47 I48 R54 E55 T56 G57 I58 F71 T72 L73 T74 I75 N76 S77 L78 T85 Y86 Y87 C88 Q89 P94 P95 G101 K107 P113 S114 V115
P120 T129 V132 L136 N137 N138 R142 Q147 V150 L154 Q155 S156 E161 S162 V163 Q166 D170 S171 T172 L175 L179 Y186 E187 Y192 T197 H198 K207 N210 E213 C214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.94Å 162.08Å 139.01Å 90.00° 98.05° 90.00°	Depositor
Resolution (Å)	42.50 – 3.19 42.50 – 3.19	Depositor EDS
% Data completeness (in resolution range)	61.0 (42.50-3.19) 61.0 (42.50-3.19)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1, BUSTER 2.11.8 (3-FEB-2022)	Depositor
R, R_{free}	0.196 , 0.310 0.197 , 0.307	Depositor DCC
R_{free} test set	855 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 88.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12316	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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	0.47	0/1636	0.72	0/2245
1	C	0.44	0/1614	0.69	0/2219
1	E	0.44	0/1567	0.68	0/2150
1	G	0.43	0/1511	0.64	0/2085
2	B	0.44	0/1584	0.67	0/2169
2	D	0.48	0/1568	0.74	0/2149
2	F	0.49	0/1578	0.76	0/2155
2	H	0.42	0/1493	0.64	0/2057
All	All	0.45	0/12551	0.69	0/17229

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1471	40	0
1	C	1576	0	1408	51	0
1	E	1533	0	1403	46	0
1	G	1477	0	1251	18	0
2	B	1551	0	1420	40	0
2	D	1535	0	1399	55	0
2	F	1547	0	1423	50	0
2	H	1461	0	1250	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	6	0	0	0	0
3	E	2	0	0	0	0
3	F	10	0	0	0	0
3	G	2	0	0	0	0
3	H	5	0	0	0	0
All	All	12316	0	11025	316	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 14.

All (316) 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:D:18:ARG:HG3	2:D:76:ASN:HA	1.37	1.06
2:B:151:ASP:HA	2:B:191:VAL:HB	1.46	0.95
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.56	0.87
2:D:19:ALA:HB3	2:D:75:ILE:HG12	1.58	0.86
2:H:54:ARG:CB	2:H:58:ILE:HB	2.07	0.83
2:B:50:GLY:HA2	2:B:91:TYR:OH	1.81	0.81
1:E:156:PRO:O	1:E:209:HIS:HE1	1.64	0.80
1:C:35:GLN:HE22	1:C:107:TRP:HE1	1.29	0.79
2:D:18:ARG:CG	2:D:76:ASN:HA	2.12	0.79
1:E:51:ILE:HG22	1:E:58:THR:HA	1.64	0.78
1:G:12:VAL:HG11	1:G:18:LEU:HD22	1.66	0.77
1:C:47:TRP:HE1	1:C:50:SER:HB2	1.51	0.75
2:F:29:VAL:CB	2:F:69:THR:HA	2.15	0.75
1:C:71:SER:HB2	1:C:80:TYR:HB2	1.68	0.75
2:D:113:PRO:HD3	2:D:198:HIS:HD2	1.49	0.75
2:D:115:VAL:HB	2:D:207:LYS:HD2	1.69	0.74
1:C:165:SER:H	1:C:206:ASN:HD21	1.33	0.74
1:E:134:ALA:HB2	1:E:220:VAL:HG12	1.69	0.74
1:C:128:PRO:HB2	1:C:151:VAL:HG12	1.70	0.73
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.71	0.72
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.70	0.72
2:D:47:LEU:HA	2:D:58:ILE:HG12	1.71	0.72
2:H:94:PRO:HB2	2:H:95:PRO:HD3	1.71	0.71
1:E:180:GLN:HB2	1:E:184:LEU:O	1.91	0.71
2:F:108:ARG:HD2	2:F:171:SER:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:THR:HB	1:G:208:ASP:HB3	1.72	0.70
2:D:163:VAL:HG22	2:D:175:LEU:HD12	1.71	0.70
1:C:64:VAL:HG13	1:C:67:ARG:HE	1.56	0.70
2:F:115:VAL:HG21	2:F:196:VAL:HG11	1.72	0.70
1:A:91:THR:HG22	1:A:120:VAL:H	1.57	0.69
2:D:15:PRO:HA	2:D:78:LEU:CB	2.22	0.69
1:C:172:VAL:HG22	1:C:191:VAL:HG12	1.75	0.68
2:H:114:SER:HB2	2:H:137:ASN:HB3	1.77	0.67
2:F:163:VAL:HG22	2:F:175:LEU:HD12	1.74	0.67
1:A:83:MET:HG2	1:A:86:LEU:HD21	1.76	0.67
1:A:153:ASP:HB3	1:A:184:LEU:HD13	1.76	0.67
1:E:128:PRO:HA	1:E:154:TYR:HB3	1.76	0.67
2:H:35:TRP:CD2	2:H:73:LEU:HD23	2.31	0.66
1:C:101:GLY:HA3	1:C:105:GLY:HA3	1.78	0.66
1:E:47:TRP:NE1	1:E:49:SER:O	2.29	0.65
2:H:142:ARG:HE	2:H:163:VAL:HG11	1.61	0.65
1:E:35:GLN:HG3	1:E:50:SER:HA	1.78	0.65
2:D:13:VAL:HG23	2:D:78:LEU:HD11	1.79	0.65
2:B:33:LEU:HD21	2:B:88:CYS:HB2	1.78	0.64
2:D:15:PRO:HA	2:D:78:LEU:HB3	1.79	0.64
2:F:33:LEU:HA	2:F:90:GLN:HA	1.79	0.64
2:D:61:ARG:NH1	2:D:62:PHE:HE1	1.95	0.63
1:C:144:THR:HG22	1:C:194:PRO:HA	1.81	0.63
2:F:148:TRP:HB2	2:F:155:GLN:HB2	1.79	0.63
1:E:35:GLN:HG2	1:E:49:SER:O	1.99	0.63
2:F:136:LEU:HD22	2:F:175:LEU:HD22	1.80	0.62
1:A:11:LEU:HD11	1:A:121:SER:HB3	1.81	0.62
1:A:36:TRP:CD1	1:A:81:LEU:HD12	2.34	0.62
1:E:68:PHE:HB3	1:E:82:GLN:O	1.99	0.62
1:E:157:GLU:HG2	1:E:158:PRO:HA	1.82	0.62
2:H:37:GLN:HB2	2:H:47:LEU:HD21	1.82	0.62
1:E:91:THR:HG22	1:E:120:VAL:H	1.64	0.61
2:B:151:ASP:CA	2:B:191:VAL:HB	2.26	0.61
1:A:193:VAL:HB	1:A:194:PRO:CD	2.30	0.61
1:G:99:ARG:HA	1:G:108:ILE:O	2.01	0.61
1:G:204:THR:HA	1:G:219:ARG:HA	1.81	0.61
1:C:163:TRP:HB3	1:C:168:LEU:HB3	1.81	0.61
2:H:48:ILE:H	2:H:54:ARG:HA	1.66	0.61
1:C:64:VAL:HG13	1:C:67:ARG:NE	2.17	0.60
1:C:64:VAL:CG1	1:C:67:ARG:HB2	2.32	0.60
1:E:70:ILE:HG13	1:E:80:TYR:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:LEU:HA	2:F:58:ILE:HG21	1.83	0.60
1:A:52:SER:HB3	1:A:57:SER:HB2	1.83	0.59
1:G:93:VAL:HA	1:G:117:LEU:HA	1.84	0.59
2:D:190:LYS:HA	2:D:211:ARG:CB	2.32	0.59
1:G:91:THR:HG23	1:G:119:THR:HA	1.83	0.59
1:G:130:VAL:HG22	1:G:151:VAL:HG23	1.85	0.59
2:F:4:LEU:HB3	2:F:25:ALA:HA	1.85	0.59
1:C:161:VAL:HG13	1:C:207:VAL:HG22	1.86	0.58
1:E:88:ALA:O	1:E:91:THR:HG23	2.02	0.58
1:E:126:LYS:HE2	1:E:153:ASP:HB3	1.85	0.58
1:G:151:VAL:HG12	1:G:187:LEU:HB3	1.85	0.58
1:A:40:ALA:HB1	1:A:41:PRO:CD	2.34	0.58
2:D:136:LEU:HD21	2:D:196:VAL:HG13	1.86	0.58
1:C:147:LEU:HB2	1:C:220:VAL:HG11	1.86	0.57
2:D:141:PRO:HD2	2:D:198:HIS:HE1	1.68	0.57
2:F:161:GLU:HB3	2:F:175:LEU:HD11	1.85	0.57
1:C:119:THR:HG21	1:C:156:PRO:HB2	1.86	0.57
1:C:159:VAL:HG23	1:C:209:HIS:HD2	1.69	0.57
2:H:210:ASN:HB2	2:H:213:GLU:HB2	1.86	0.57
1:E:174:THR:HG23	1:E:189:SER:HB2	1.87	0.56
2:F:59:PRO:HB2	2:F:61:ARG:HD2	1.87	0.56
1:C:119:THR:HG21	1:C:156:PRO:CB	2.36	0.56
2:D:113:PRO:HD3	2:D:198:HIS:CD2	2.38	0.56
2:D:124:GLN:HE22	2:D:131:SER:HB3	1.69	0.56
1:E:153:ASP:OD1	1:E:180:GLN:NE2	2.33	0.56
1:C:165:SER:H	1:C:206:ASN:ND2	2.03	0.56
1:E:88:ALA:HA	1:E:120:VAL:HB	1.87	0.56
2:H:33:LEU:HA	2:H:89:GLN:O	2.05	0.56
1:C:173:HIS:CE1	2:D:137:ASN:ND2	2.74	0.56
2:B:151:ASP:OD2	2:B:189:HIS:HD2	1.89	0.55
1:C:32:TYR:CE2	1:C:98:ARG:NH1	2.74	0.55
2:D:61:ARG:HH11	2:D:62:PHE:HE1	1.53	0.55
2:H:15:PRO:HA	2:H:78:LEU:HB3	1.88	0.55
1:C:20:LEU:HD11	1:C:118:VAL:HG21	1.88	0.54
1:A:35:GLN:HB3	1:A:50:SER:HA	1.88	0.54
1:E:156:PRO:O	1:E:209:HIS:CE1	2.53	0.54
2:B:158:ASN:HD22	2:B:159:SER:N	2.05	0.54
1:A:128:PRO:HB3	1:A:154:TYR:HB3	1.89	0.54
2:B:108:ARG:HG2	2:B:109:THR:H	1.72	0.54
2:B:2:ILE:O	2:B:97:THR:HG21	2.08	0.54
2:B:108:ARG:HG2	2:B:109:THR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:PRO:HD3	2:D:164:THR:HG22	1.90	0.54
2:D:108:ARG:HD3	2:D:109:THR:O	2.08	0.54
2:F:175:LEU:HG	2:F:176:SER:N	2.23	0.54
1:E:209:HIS:HD2	1:E:212:SER:CB	2.21	0.54
2:F:113:PRO:HD3	2:F:198:HIS:HD2	1.73	0.54
2:D:112:ALA:HA	2:D:200:GLY:HA3	1.89	0.54
1:G:165:SER:H	1:G:206:ASN:HD21	1.54	0.54
1:A:40:ALA:HB3	1:A:43:LYS:HB3	1.90	0.53
1:C:162:SER:HB2	1:C:206:ASN:HB2	1.91	0.53
2:H:35:TRP:CG	2:H:73:LEU:HD23	2.44	0.53
2:H:154:LEU:HD23	2:H:156:SER:HB2	1.91	0.53
2:D:148:TRP:HD1	2:D:159:SER:HB3	1.73	0.53
2:F:4:LEU:HD22	2:F:4:LEU:H	1.73	0.53
2:H:35:TRP:CE2	2:H:73:LEU:HD23	2.44	0.53
2:B:165:GLU:O	2:B:166:GLN:O	2.27	0.53
2:D:100:GLY:O	2:D:101:GLY:O	2.27	0.53
1:C:174:THR:HG1	1:C:189:SER:HG	1.56	0.52
2:D:37:GLN:CB	2:D:47:LEU:HD21	2.39	0.52
2:D:148:TRP:CD1	2:D:159:SER:HB3	2.45	0.52
1:G:191:VAL:HG12	1:G:193:VAL:HG13	1.90	0.52
2:B:193:ALA:HB2	2:B:208:SER:CB	2.39	0.52
1:A:89:GLU:OE2	1:A:90:ASP:OD1	2.28	0.52
1:A:194:PRO:HG2	1:A:197:SER:HB3	1.92	0.51
2:B:112:ALA:HB2	2:B:200:GLY:HA3	1.92	0.51
2:D:37:GLN:HB2	2:D:47:LEU:HD21	1.92	0.51
1:C:186:SER:O	1:C:187:LEU:HB2	2.11	0.51
2:F:25:ALA:HB3	2:F:69:THR:HG22	1.93	0.51
1:E:163:TRP:HD1	1:E:172:VAL:HG11	1.75	0.51
2:F:186:TYR:O	2:F:192:TYR:OH	2.29	0.51
2:B:6:GLN:HE22	2:B:87:TYR:HA	1.74	0.51
1:E:16:GLY:O	1:E:83:MET:O	2.29	0.51
1:G:13:GLN:HB2	1:G:14:PRO:HD2	1.93	0.51
2:H:36:TYR:HB3	2:H:44:PRO:HB2	1.92	0.51
2:D:3:VAL:HB	2:D:26:SER:HB2	1.93	0.50
1:A:131:PHE:CE2	2:B:124:GLN:HG3	2.46	0.50
1:E:194:PRO:HG2	1:E:197:SER:HB2	1.92	0.50
2:F:186:TYR:CE2	2:F:211:ARG:HG3	2.46	0.50
1:A:4:LEU:HA	1:A:24:ALA:HB2	1.94	0.50
2:D:114:SER:O	2:D:136:LEU:HA	2.12	0.50
1:G:164:ASN:HB2	1:G:167:ALA:HB3	1.93	0.50
1:C:98:ARG:NH2	1:C:111:TYR:CE2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:PRO:HG3	2:F:106:ILE:HG22	1.94	0.50
2:F:148:TRP:CE2	2:F:179:LEU:HB2	2.47	0.50
2:F:37:GLN:HB2	2:F:47:LEU:CD1	2.37	0.50
2:F:6:GLN:HE22	2:F:87:TYR:HA	1.75	0.50
2:B:38:GLN:HE21	2:B:44:PRO:HD3	1.75	0.49
2:D:81:GLU:HA	2:D:168:SER:HA	1.93	0.49
2:F:182:SER:HB2	2:F:185:ASP:HB2	1.94	0.49
1:E:45:LEU:HD11	2:F:44:PRO:HG3	1.92	0.49
1:C:5:VAL:O	1:C:22:CYS:HA	2.13	0.49
2:F:15:PRO:HD3	2:F:107:LYS:O	2.12	0.49
1:E:36:TRP:NE1	1:E:81:LEU:HB2	2.27	0.49
1:E:209:HIS:HD2	1:E:212:SER:OG	1.96	0.49
2:D:15:PRO:HA	2:D:78:LEU:HB2	1.95	0.49
1:C:71:SER:CB	1:C:80:TYR:HB2	2.41	0.49
2:F:6:GLN:NE2	2:F:88:CYS:SG	2.86	0.49
1:E:174:THR:HA	1:E:189:SER:HA	1.94	0.48
2:F:62:PHE:HE1	2:F:75:ILE:HD12	1.78	0.48
1:A:36:TRP:CG	1:A:81:LEU:HD13	2.47	0.48
1:C:46:GLU:HG3	1:C:61:ARG:HH12	1.79	0.48
1:C:99:ARG:NH1	1:C:107:TRP:CZ3	2.81	0.48
1:A:39:GLN:O	1:A:40:ALA:O	2.30	0.48
2:D:33:LEU:HD11	2:D:88:CYS:HB2	1.95	0.48
2:H:86:TYR:O	2:H:101:GLY:HA2	2.13	0.48
2:B:35:TRP:CG	2:B:73:LEU:HD13	2.49	0.48
1:G:128:PRO:HB2	1:G:151:VAL:HG22	1.96	0.48
1:C:145:ALA:HB3	1:C:198:LEU:HD21	1.96	0.48
1:C:130:VAL:HB	1:C:151:VAL:HG13	1.95	0.48
1:C:174:THR:OG1	1:C:189:SER:OG	2.31	0.48
2:D:18:ARG:HG3	2:D:76:ASN:CA	2.26	0.48
1:A:91:THR:CG2	1:A:120:VAL:H	2.25	0.47
2:B:181:LEU:HD11	2:B:185:ASP:HB2	1.95	0.47
2:B:12:SER:HA	2:B:105:GLU:O	2.14	0.47
1:A:36:TRP:CD1	1:A:81:LEU:CD1	2.97	0.47
2:B:103:LYS:HE2	2:B:105:GLU:HB2	1.96	0.47
1:C:39:GLN:HG3	1:C:45:LEU:HD23	1.95	0.47
1:E:177:ALA:HB2	1:E:187:LEU:HD23	1.95	0.47
1:C:159:VAL:HG23	1:C:209:HIS:CD2	2.49	0.47
2:D:146:VAL:HG21	2:D:177:SER:HB2	1.96	0.47
2:F:89:GLN:HA	2:F:98:PHE:HA	1.95	0.47
2:F:189:HIS:O	2:F:211:ARG:HD2	2.14	0.47
2:H:147:GLN:HE21	2:H:154:LEU:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:THR:HA	1:E:218:LYS:O	2.14	0.47
1:A:174:THR:HG23	1:A:187:LEU:HD13	1.96	0.47
2:D:151:ASP:OD1	2:D:191:VAL:HG23	2.15	0.47
2:F:6:GLN:HB3	2:F:102:THR:HG23	1.97	0.47
2:F:161:GLU:HG2	2:F:175:LEU:HD21	1.97	0.46
1:C:98:ARG:HH21	1:C:111:TYR:HE2	1.63	0.46
2:D:20:THR:HA	2:D:74:THR:HG22	1.96	0.46
1:E:197:SER:HA	1:E:200:THR:OG1	2.15	0.46
1:A:18:LEU:HD21	1:A:118:VAL:HG13	1.97	0.46
2:B:113:PRO:HB3	2:B:139:PHE:CD1	2.49	0.46
2:F:2:ILE:HG23	2:F:26:SER:HB2	1.96	0.46
2:H:1:GLU:O	2:H:2:ILE:O	2.33	0.46
2:B:138:ASN:OD1	2:B:174:SER:OG	2.34	0.46
1:E:48:VAL:HG13	1:E:64:VAL:HG21	1.98	0.46
2:B:33:LEU:H	2:B:51:ALA:HB2	1.80	0.46
2:D:86:TYR:O	2:D:101:GLY:HA2	2.14	0.46
1:E:38:ARG:HD3	1:E:94:TYR:OH	2.16	0.46
2:F:4:LEU:HD23	2:F:99:GLY:HA2	1.97	0.46
1:C:172:VAL:HG22	1:C:191:VAL:CG1	2.45	0.46
1:G:10:GLY:HA3	1:G:118:VAL:HA	1.98	0.46
2:H:161:GLU:HG2	2:H:175:LEU:HD11	1.98	0.46
1:C:173:HIS:CE1	2:D:137:ASN:HD22	2.34	0.46
2:B:136:LEU:HD11	2:B:146:VAL:HG22	1.98	0.45
2:F:38:GLN:HG3	2:F:42:GLN:O	2.16	0.45
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.97	0.45
2:F:197:THR:HG22	2:F:204:PRO:HB3	1.98	0.45
2:B:2:ILE:HG23	2:B:27:ARG:H	1.82	0.45
2:B:158:ASN:HD22	2:B:159:SER:H	1.63	0.45
2:D:193:ALA:HB1	2:D:206:THR:HG23	1.98	0.45
1:A:154:TYR:O	1:A:155:PHE:HB2	2.17	0.45
1:C:21:SER:HA	1:C:80:TYR:HA	1.99	0.45
2:D:107:LYS:HZ2	2:D:140:TYR:HE1	1.65	0.45
1:E:6:GLU:HG3	1:E:115:GLY:H	1.82	0.45
1:A:34:ILE:CG2	1:A:79:LEU:HD22	2.46	0.45
1:C:209:HIS:HB3	1:C:214:THR:OG1	2.16	0.45
1:E:34:ILE:HD13	1:E:98:ARG:HB3	1.99	0.45
1:E:163:TRP:CD1	1:E:172:VAL:CG1	3.00	0.45
2:F:166:GLN:HE21	2:F:171:SER:HB3	1.81	0.45
1:G:94:TYR:O	1:G:115:GLY:HA2	2.16	0.45
2:D:166:GLN:HG3	2:D:171:SER:HA	1.99	0.45
2:D:201:LEU:HG	2:D:205:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:TYR:O	2:B:101:GLY:HA2	2.17	0.45
1:E:177:ALA:HA	1:E:187:LEU:HB3	1.98	0.45
2:F:61:ARG:HD2	2:F:61:ARG:H	1.82	0.44
1:A:6:GLU:HA	1:A:22:CYS:HA	2.00	0.44
1:A:36:TRP:HD1	1:A:70:ILE:CD1	2.31	0.44
2:B:66:GLY:HA3	2:B:70:ASP:O	2.17	0.44
2:F:39:LYS:HG2	2:F:84:ALA:HB2	1.98	0.44
1:E:130:VAL:HG12	1:E:218:LYS:HD3	1.99	0.44
1:E:163:TRP:HD1	1:E:172:VAL:CG1	2.30	0.44
1:A:154:TYR:HE1	1:A:157:GLU:HA	1.82	0.44
2:B:35:TRP:CB	2:B:73:LEU:HD13	2.48	0.44
1:C:190:VAL:HG21	2:D:135:LEU:CD2	2.47	0.44
2:B:83:ALA:HB2	2:B:106:ILE:HD11	2.00	0.44
2:B:107:LYS:HA	2:B:140:TYR:OH	2.18	0.44
2:B:148:TRP:CZ3	2:B:194:CYS:HB3	2.53	0.44
2:D:61:ARG:NH1	2:D:62:PHE:CE1	2.80	0.43
1:E:5:VAL:HB	1:E:23:ALA:HB3	1.99	0.43
1:C:173:HIS:HE1	2:D:137:ASN:ND2	2.15	0.43
1:E:108:ILE:O	2:F:36:TYR:OH	2.28	0.43
1:A:64:VAL:HG13	1:A:68:PHE:HB2	2.01	0.43
1:E:49:SER:OG	1:E:70:ILE:HG21	2.19	0.43
1:A:133:LEU:HB3	2:B:118:PHE:HB3	1.99	0.43
1:E:99:ARG:HA	1:E:109:PHE:H	1.84	0.43
2:B:198:HIS:CD2	2:B:200:GLY:H	2.36	0.43
1:C:70:ILE:HA	1:C:81:LEU:HD12	2.00	0.43
2:D:24:ARG:HD3	2:F:126:LYS:NZ	2.34	0.43
2:D:136:LEU:HD11	2:D:196:VAL:HG22	2.00	0.43
2:D:141:PRO:HD2	2:D:198:HIS:CE1	2.51	0.43
1:A:40:ALA:HB3	1:A:43:LYS:CB	2.48	0.43
1:A:68:PHE:N	1:A:68:PHE:CD1	2.87	0.43
1:E:163:TRP:CD1	1:E:172:VAL:HG13	2.53	0.43
1:A:176:PRO:HG2	2:B:163:VAL:O	2.19	0.42
1:A:193:VAL:HB	1:A:194:PRO:HD3	2.00	0.42
2:D:47:LEU:CA	2:D:58:ILE:HG12	2.45	0.42
2:D:115:VAL:HG22	2:D:196:VAL:HG21	2.01	0.42
2:F:90:GLN:O	2:F:96:GLY:HA3	2.19	0.42
1:C:93:VAL:HG22	1:C:117:LEU:HD12	2.01	0.42
2:D:19:ALA:HB3	2:D:75:ILE:CG1	2.38	0.42
1:C:64:VAL:HG22	1:C:67:ARG:HH21	1.84	0.42
1:E:60:TYR:CE1	1:E:70:ILE:HG22	2.55	0.42
1:E:125:THR:HG21	1:E:211:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:VAL:HG13	2:F:175:LEU:HB2	2.01	0.42
2:H:113:PRO:HD3	2:H:198:HIS:HD2	1.83	0.42
2:H:136:LEU:HD22	2:H:175:LEU:HD23	2.02	0.42
2:D:190:LYS:O	2:D:210:ASN:HA	2.17	0.42
2:F:14:SER:HB2	2:F:17:GLU:OE1	2.19	0.42
2:F:49:TYR:O	2:F:53:THR:OG1	2.25	0.42
1:G:11:LEU:HD22	1:G:211:PRO:HB3	2.01	0.42
1:A:146:ALA:HB2	1:A:192:THR:HG22	2.02	0.42
2:F:38:GLN:CG	2:F:42:GLN:O	2.68	0.42
1:C:64:VAL:HG12	1:C:67:ARG:HB2	1.98	0.42
1:E:100:THR:HG22	1:E:101:GLY:H	1.84	0.42
2:D:116:PHE:HB2	2:D:135:LEU:HB3	2.01	0.42
2:D:155:GLN:O	2:D:158:ASN:OD1	2.38	0.42
2:F:39:LYS:O	2:F:42:GLN:HB2	2.20	0.42
2:H:35:TRP:CD1	2:H:73:LEU:HD23	2.55	0.41
2:H:115:VAL:HB	2:H:207:LYS:HG3	2.01	0.41
1:C:128:PRO:HB2	1:C:151:VAL:CG1	2.46	0.41
1:A:68:PHE:N	1:A:68:PHE:HD1	2.17	0.41
1:C:7:SER:HB3	1:C:21:SER:H	1.85	0.41
2:F:6:GLN:NE2	2:F:88:CYS:H	2.18	0.41
2:F:58:ILE:HA	2:F:59:PRO:HD3	1.92	0.41
1:A:164:ASN:HB3	1:A:167:ALA:HB3	2.03	0.41
2:D:113:PRO:HB3	2:D:139:PHE:HB3	2.02	0.41
2:F:113:PRO:HB3	2:F:139:PHE:CD2	2.56	0.41
1:A:17:SER:OG	1:A:83:MET:O	2.24	0.41
1:A:52:SER:CB	1:A:57:SER:HB2	2.49	0.41
1:A:87:ARG:O	1:A:120:VAL:HG21	2.20	0.41
1:A:40:ALA:HB1	1:A:41:PRO:HD3	2.02	0.41
2:B:128:GLY:O	2:B:183:LYS:HB2	2.20	0.41
1:E:92:ALA:O	1:E:118:VAL:HB	2.20	0.41
1:A:22:CYS:HB3	1:A:79:LEU:HB3	2.02	0.41
1:G:161:VAL:HG22	1:G:207:VAL:HG12	2.03	0.41
1:C:117:LEU:HD22	1:C:158:PRO:HD3	2.02	0.40
2:B:15:PRO:HD3	2:B:107:LYS:O	2.20	0.40
2:H:150:VAL:CG2	2:H:155:GLN:HG3	2.51	0.40
2:H:150:VAL:HG23	2:H:155:GLN:HG3	2.03	0.40
1:C:164:ASN:HB2	1:C:168:LEU:HB2	2.04	0.40
2:H:186:TYR:HA	2:H:192:TYR:OH	2.21	0.40
2:B:6:GLN:NE2	2:B:99:GLY:HA3	2.36	0.40
2:B:13:VAL:HG12	2:B:78:LEU:HD22	2.02	0.40
2:B:190:LYS:O	2:B:210:ASN:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:HB2	1:C:61:ARG:HH12	1.86	0.40
2:F:135:LEU:HD22	2:F:137:ASN:HB2	2.03	0.40
1:G:39:GLN:O	1:G:39:GLN:HG3	2.22	0.40
2:H:19:ALA:H	2:H:75:ILE:CB	2.33	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	220/227 (97%)	178 (81%)	37 (17%)	5 (2%)	6 34
1	C	221/227 (97%)	183 (83%)	28 (13%)	10 (4%)	2 18
1	E	212/227 (93%)	186 (88%)	23 (11%)	3 (1%)	11 46
1	G	216/227 (95%)	186 (86%)	27 (12%)	3 (1%)	11 46
2	B	212/214 (99%)	179 (84%)	27 (13%)	6 (3%)	5 29
2	D	212/214 (99%)	177 (84%)	26 (12%)	9 (4%)	3 20
2	F	212/214 (99%)	168 (79%)	29 (14%)	15 (7%)	1 8
2	H	212/214 (99%)	185 (87%)	18 (8%)	9 (4%)	3 20
All	All	1717/1764 (97%)	1442 (84%)	215 (12%)	60 (4%)	3 24

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
2	B	166	GLN
1	C	7	SER
1	C	29	PHE
1	C	56	GLN
2	D	101	GLY

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Mol	Chain	Res	Type
2	D	154	LEU
2	D	166	GLN
2	D	195	GLU
1	E	138	ARG
1	E	153	ASP
2	F	29	VAL
2	F	138	ASN
1	G	156	PRO
2	H	2	ILE
2	H	56	THR
2	H	107	LYS
1	A	16	GLY
1	A	17	SER
1	A	40	ALA
2	B	95	PRO
2	B	138	ASN
1	C	33	ASP
1	C	41	PRO
1	C	153	ASP
2	D	30	ARG
2	D	110	VAL
2	F	40	PRO
2	F	99	GLY
2	F	107	LYS
2	F	110	VAL
2	F	211	ARG
2	H	138	ASN
1	A	7	SER
2	B	143	GLU
2	B	158	ASN
1	C	106	GLY
2	D	138	ASN
2	F	26	SER
2	F	31	ARG
2	F	52	SER
2	F	69	THR
2	F	158	ASN
2	H	48	ILE
2	H	170	ASP
1	C	8	GLY
2	D	51	ALA
1	E	158	PRO

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Mol	Chain	Res	Type
2	F	33	LEU
2	F	70	ASP
2	F	213	GLU
1	G	7	SER
1	G	158	PRO
2	H	76	ASN
2	B	42	GLN
1	C	184	LEU
1	C	187	LEU
2	H	166	GLN
2	H	94	PRO
2	D	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	165/193 (86%)	146 (88%)	19 (12%)	5 24
1	C	161/193 (83%)	140 (87%)	21 (13%)	4 19
1	E	158/193 (82%)	145 (92%)	13 (8%)	11 41
1	G	139/193 (72%)	114 (82%)	25 (18%)	1 9
2	B	162/182 (89%)	139 (86%)	23 (14%)	3 15
2	D	159/182 (87%)	133 (84%)	26 (16%)	2 11
2	F	162/182 (89%)	136 (84%)	26 (16%)	2 11
2	H	139/182 (76%)	120 (86%)	19 (14%)	3 17
All	All	1245/1500 (83%)	1073 (86%)	172 (14%)	3 16

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	11	LEU
1	A	18	LEU

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Mol	Chain	Res	Type
1	A	35	GLN
1	A	43	LYS
1	A	63	GLU
1	A	68	PHE
1	A	74	ASN
1	A	78	THR
1	A	83	MET
1	A	89	GLU
1	A	117	LEU
1	A	122	SER
1	A	124	SER
1	A	125	THR
1	A	129	SER
1	A	164	ASN
1	A	198	LEU
1	A	218	LYS
2	B	7	SER
2	B	11	LEU
2	B	14	SER
2	B	21	LEU
2	B	33	LEU
2	B	53	THR
2	B	58	ILE
2	B	65	SER
2	B	72	THR
2	B	76	ASN
2	B	85	THR
2	B	92	ARG
2	B	93	ASP
2	B	106	ILE
2	B	125	LEU
2	B	143	GLU
2	B	150	VAL
2	B	154	LEU
2	B	158	ASN
2	B	159	SER
2	B	175	LEU
2	B	177	SER
2	B	183	LYS
1	C	11	LEU
1	C	28	THR
1	C	33	ASP

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Mol	Chain	Res	Type
1	C	35	GLN
1	C	45	LEU
1	C	78	THR
1	C	98	ARG
1	C	99	ARG
1	C	107	TRP
1	C	116	THR
1	C	117	LEU
1	C	125	THR
1	C	129	SER
1	C	138	ARG
1	C	147	LEU
1	C	155	PHE
1	C	159	VAL
1	C	179	LEU
1	C	187	LEU
1	C	195	SER
1	C	214	THR
2	D	5	THR
2	D	13	VAL
2	D	18	ARG
2	D	21	LEU
2	D	22	SER
2	D	29	VAL
2	D	42	GLN
2	D	47	LEU
2	D	53	THR
2	D	65	SER
2	D	69	THR
2	D	74	THR
2	D	75	ILE
2	D	97	THR
2	D	108	ARG
2	D	152	ASN
2	D	154	LEU
2	D	159	SER
2	D	163	VAL
2	D	166	GLN
2	D	172	THR
2	D	185	ASP
2	D	191	VAL
2	D	197	THR

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Mol	Chain	Res	Type
2	D	203	SER
2	D	210	ASN
1	E	12	VAL
1	E	21	SER
1	E	37	VAL
1	E	51	ILE
1	E	68	PHE
1	E	81	LEU
1	E	82	GLN
1	E	110	ASP
1	E	149	CYS
1	E	162	SER
1	E	169	THR
1	E	192	THR
1	E	206	ASN
2	F	1	GLU
2	F	4	LEU
2	F	26	SER
2	F	48	ILE
2	F	52	SER
2	F	53	THR
2	F	55	GLU
2	F	56	THR
2	F	61	ARG
2	F	63	SER
2	F	65	SER
2	F	75	ILE
2	F	78	LEU
2	F	85	THR
2	F	114	SER
2	F	135	LEU
2	F	154	LEU
2	F	163	VAL
2	F	164	THR
2	F	167	ASP
2	F	172	THR
2	F	175	LEU
2	F	177	SER
2	F	178	THR
2	F	179	LEU
2	F	182	SER
1	G	1	GLN

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Mol	Chain	Res	Type
1	G	4	LEU
1	G	11	LEU
1	G	13	GLN
1	G	18	LEU
1	G	32	TYR
1	G	39	GLN
1	G	45	LEU
1	G	59	TYR
1	G	70	ILE
1	G	76	LYS
1	G	118	VAL
1	G	119	THR
1	G	129	SER
1	G	144	THR
1	G	149	CYS
1	G	150	LEU
1	G	151	VAL
1	G	162	SER
1	G	165	SER
1	G	187	LEU
1	G	200	THR
1	G	206	ASN
1	G	213	ASN
1	G	217	ASP
2	H	13	VAL
2	H	17	GLU
2	H	21	LEU
2	H	23	CYS
2	H	42	GLN
2	H	47	LEU
2	H	71	PHE
2	H	73	LEU
2	H	78	LEU
2	H	85	THR
2	H	88	CYS
2	H	115	VAL
2	H	129	THR
2	H	147	GLN
2	H	172	THR
2	H	179	LEU
2	H	187	GLU
2	H	197	THR

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Mol	Chain	Res	Type
2	H	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	206	ASN
2	B	6	GLN
2	B	38	GLN
2	B	158	ASN
2	B	189	HIS
2	B	198	HIS
1	C	173	HIS
1	C	206	ASN
2	D	137	ASN
2	D	152	ASN
2	D	158	ASN
2	D	189	HIS
1	E	209	HIS
2	F	6	GLN
2	F	137	ASN
2	F	155	GLN
2	F	198	HIS
2	F	199	GLN
2	F	210	ASN
1	G	74	ASN
1	G	206	ASN
2	H	147	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	222/227 (97%)	-0.55	1 (0%) 91 86	14, 47, 71, 84	0
1	C	223/227 (98%)	-0.50	0 100 100	35, 56, 68, 80	0
1	E	216/227 (95%)	-0.49	0 100 100	26, 53, 64, 74	0
1	G	220/227 (96%)	-0.33	1 (0%) 91 86	51, 76, 88, 90	0
2	B	214/214 (100%)	-0.62	0 100 100	22, 46, 71, 78	0
2	D	214/214 (100%)	-0.62	0 100 100	17, 39, 63, 76	0
2	F	214/214 (100%)	-0.59	0 100 100	17, 41, 64, 70	0
2	H	214/214 (100%)	-0.37	0 100 100	37, 63, 85, 89	0
All	All	1737/1764 (98%)	-0.51	2 (0%) 95 95	14, 53, 82, 90	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	SER	2.7
1	G	112	TRP	2.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.