



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:39 AM UTC

PDB ID : 8GV0 / pdb_00008gv0
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

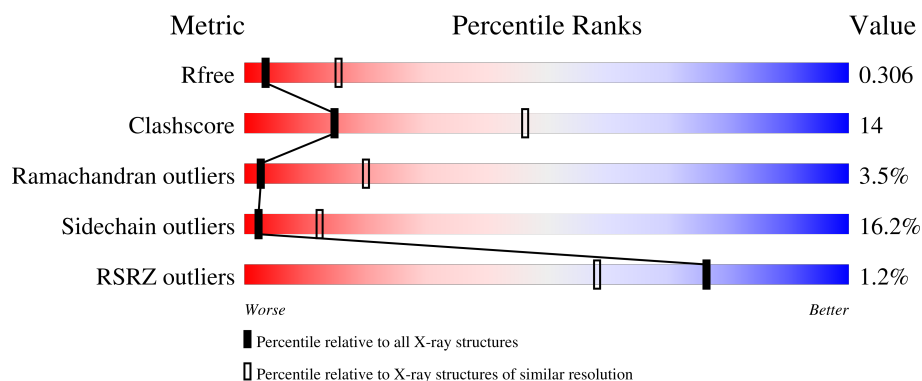
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	 64% 28% 5% ..
1	C	227	 63% 29% 7% .
1	E	227	 59% 32% . 5%
1	G	227	 73% 21% . .
2	B	214	 61% 34% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	214	57% 36% 7%
2	F	214	% 56% 34% 9%
2	H	214	3% 69% 27%

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		

Continued on next page...

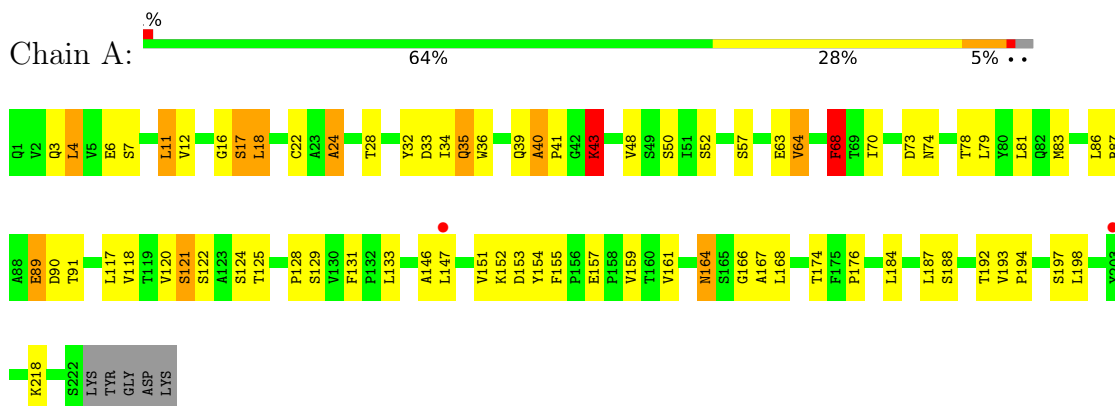
Continued from previous page...

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

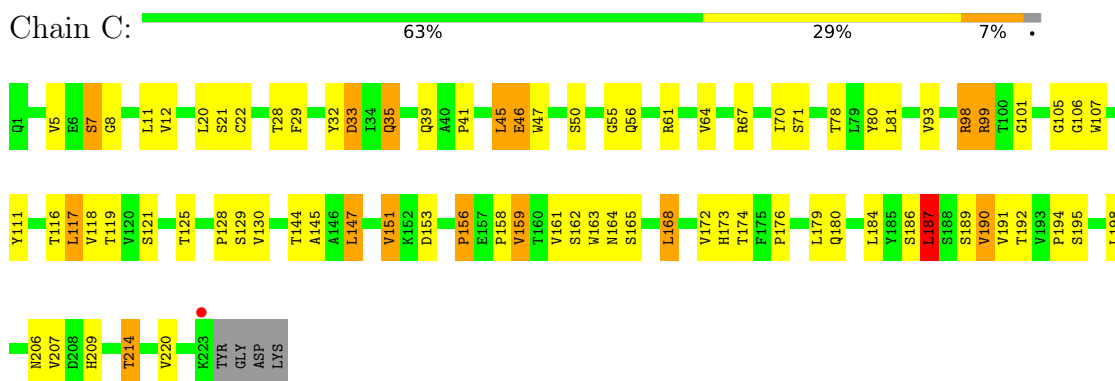
3 Residue-property plots [i](#)

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.

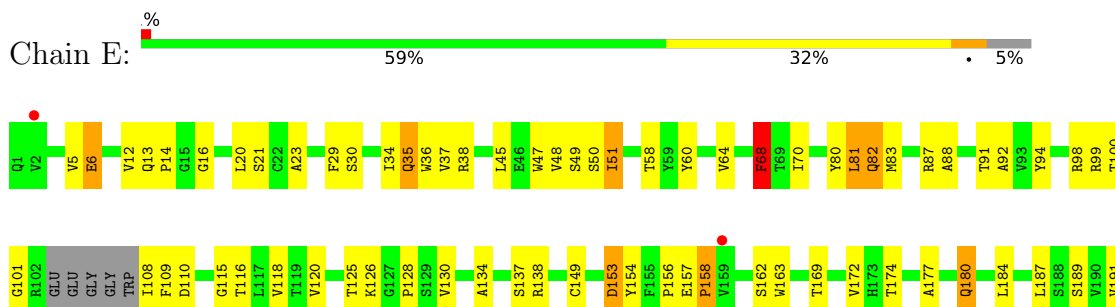
- Molecule 1: Anti-factor IXa IgG fab heavy chain



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

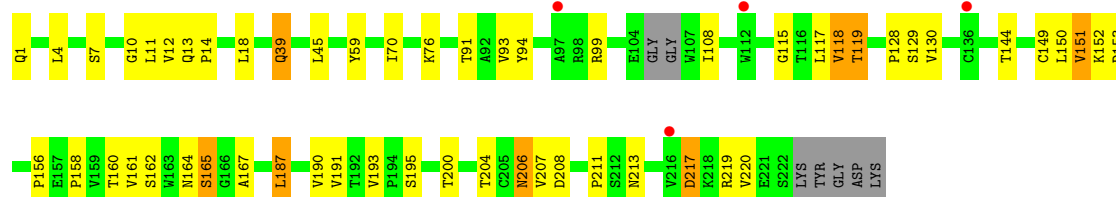
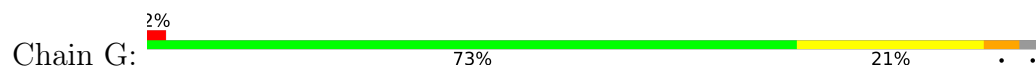


- Molecule 1: Anti-factor IXa IgG fab heavy chain

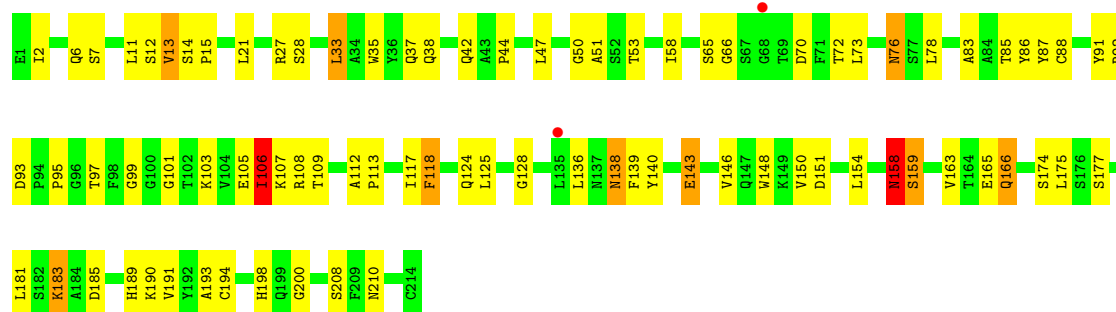




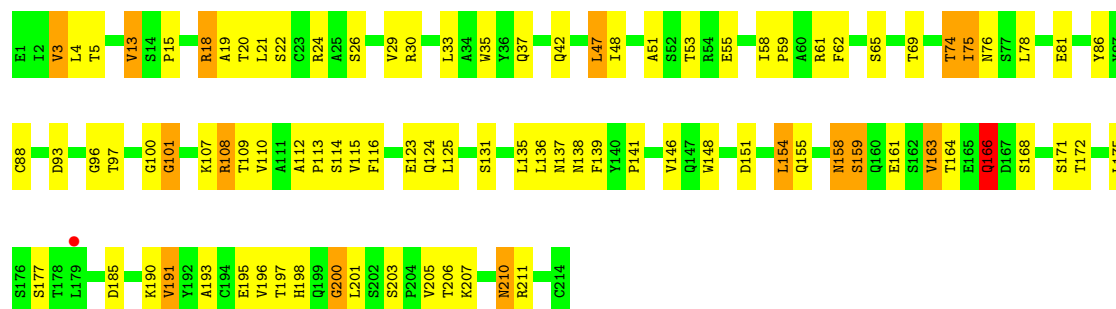
• Molecule 1: Anti-factor IXa IgG fab heavy chain



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

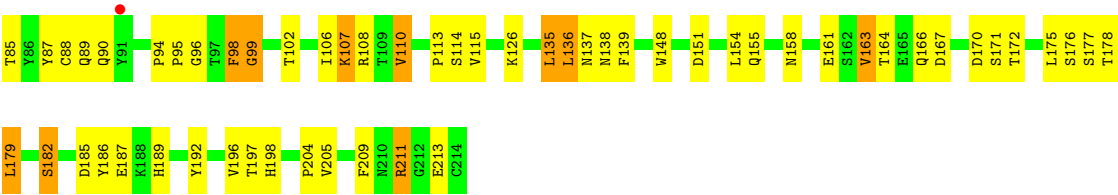


• Molecule 2: Anti-factor IXa IgG fab light chain

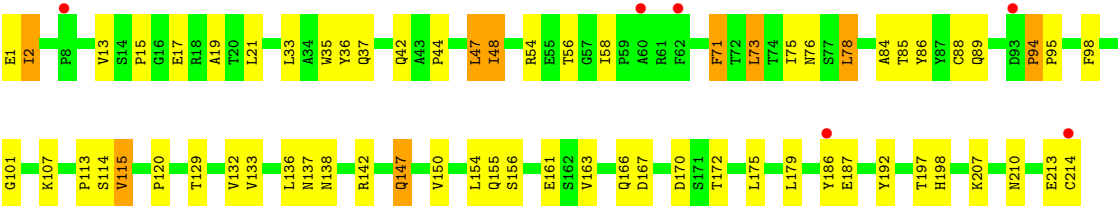


• Molecule 2: Anti-factor IXa IgG fab light chain





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 0.194 , 0.306	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)	0.30 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.86	0/1636	1.29	12/2245 (0.5%)
1	C	0.80	0/1614	1.17	8/2219 (0.4%)
1	E	0.82	1/1567 (0.1%)	1.16	7/2150 (0.3%)
1	G	0.84	0/1511	1.14	4/2085 (0.2%)
2	B	0.80	0/1584	1.18	3/2169 (0.1%)
2	D	0.85	0/1568	1.29	7/2149 (0.3%)
2	F	0.88	0/1578	1.33	10/2155 (0.5%)
2	H	0.81	1/1493 (0.1%)	1.14	3/2057 (0.1%)
All	All	0.83	2/12551 (0.0%)	1.21	54/17229 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	137	SER	CA-C	6.59	1.57	1.53
2	H	84	ALA	CA-C	5.00	1.59	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	ASP	CA-CB-CG	11.35	123.95	112.60
1	A	151	VAL	CA-C-N	9.20	133.58	120.79
1	A	151	VAL	C-N-CA	9.20	133.58	120.79
2	F	209	PHE	CA-CB-CG	8.46	122.25	113.80
1	A	152	LYS	N-CA-C	7.27	119.88	111.02
1	C	121	SER	CA-C-N	7.27	130.02	120.28
1	C	121	SER	C-N-CA	7.27	130.02	120.28
1	A	28	THR	CA-C-N	6.58	129.09	120.28
1	A	28	THR	C-N-CA	6.58	129.09	120.28
2	B	76	ASN	CA-CB-CG	6.50	119.10	112.60
1	G	217	ASP	CA-CB-CG	6.26	118.86	112.60
2	D	158	ASN	CA-C-N	6.04	130.46	122.30
2	D	158	ASN	C-N-CA	6.04	130.46	122.30
2	D	123	GLU	N-CA-C	-6.00	105.62	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ALA	N-CA-C	5.86	118.77	108.75
1	C	55	GLY	CA-C-N	5.85	132.72	121.54
1	C	55	GLY	C-N-CA	5.85	132.72	121.54
1	E	206	ASN	CA-CB-CG	5.71	118.31	112.60
1	E	68	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	33	ASP	CA-CB-CG	5.64	118.24	112.60
2	F	170	ASP	CA-CB-CG	5.62	118.22	112.60
1	E	29	PHE	CA-C-N	5.62	127.81	120.28
1	E	29	PHE	C-N-CA	5.62	127.81	120.28
1	G	152	LYS	N-CA-C	5.61	117.62	108.76
2	D	96	GLY	N-CA-C	5.55	119.08	111.54
2	F	151	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	200	GLY	CA-C-N	5.45	129.87	122.19
2	D	200	GLY	C-N-CA	5.45	129.87	122.19
1	C	180	GLN	CA-C-N	5.41	127.84	120.54
1	C	180	GLN	C-N-CA	5.41	127.84	120.54
2	B	106	ILE	N-CA-CB	5.38	116.98	110.95
1	A	121	SER	CA-C-N	5.38	128.03	120.28
1	A	121	SER	C-N-CA	5.38	128.03	120.28
1	E	30	SER	N-CA-C	5.34	117.11	111.28
2	B	118	PHE	CA-CB-CG	-5.34	108.46	113.80
2	F	187	GLU	CA-C-N	5.32	129.12	120.60
2	F	187	GLU	C-N-CA	5.32	129.12	120.60
2	F	41	GLY	CA-C-N	5.28	128.58	120.82
2	F	41	GLY	C-N-CA	5.28	128.58	120.82
1	A	68	PHE	CA-CB-CG	5.26	119.06	113.80
2	F	98	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	32	TYR	N-CA-C	5.17	118.17	109.95
2	H	98	PHE	N-CA-C	5.16	118.01	109.85
2	F	34	ALA	CA-C-N	5.15	130.67	122.74
2	F	34	ALA	C-N-CA	5.15	130.67	122.74
1	E	180	GLN	CA-C-N	5.13	127.41	120.38
1	E	180	GLN	C-N-CA	5.13	127.41	120.38
1	C	156	PRO	CA-C-N	5.12	127.34	120.58
1	C	156	PRO	C-N-CA	5.12	127.34	120.58
1	G	195	SER	CA-C-N	5.10	127.83	120.38
1	G	195	SER	C-N-CA	5.10	127.83	120.38
2	H	71	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	73	ASP	CA-CB-CG	5.07	117.67	112.60
2	H	167	ASP	CA-CB-CG	5.06	117.66	112.60

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	42	0
1	C	1576	0	1408	53	0
1	E	1533	0	1403	47	0
1	G	1477	0	1251	18	0
2	B	1551	0	1420	40	0
2	D	1535	0	1399	54	0
2	F	1547	0	1423	51	0
2	H	1461	0	1250	27	0
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	321	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 (321) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:35:GLN:HE22	1:C:107:TRP:NE1	1.88	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:17:SER:OG	1:A:83:MET:O	2.24	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:83:MET:HE2	1:A:118:VAL:HG11	1.95	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:C:162:SER:C	1:C:206:ASN:HD22	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:39:LYS:O	2:F:40:PRO:C	2.61	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:ASN:C	1:A:166:GLY:H	2.28	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:E:13:GLN:O	1:E:14:PRO:C	2.64	0.41
1:G:161:VAL:HG22	1:G:207:VAL:HG12	2.03	0.41
2:F:94:PRO:HA	2:F:95:PRO:C	2.46	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
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%)	5	29
1	C	221/227 (97%)	183 (83%)	28 (13%)	10 (4%)	2	15
1	E	212/227 (93%)	186 (88%)	23 (11%)	3 (1%)	9	39
1	G	216/227 (95%)	186 (86%)	27 (12%)	3 (1%)	9	39
2	B	212/214 (99%)	179 (84%)	27 (13%)	6 (3%)	4	25
2	D	212/214 (99%)	177 (84%)	26 (12%)	9 (4%)	2	16
2	F	212/214 (99%)	168 (79%)	29 (14%)	15 (7%)	1	6
2	H	212/214 (99%)	185 (87%)	18 (8%)	9 (4%)	2	16
All	All	1717/1764 (97%)	1442 (84%)	215 (12%)	60 (4%)	3	20

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 ⓘ

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%)	138 (84%)	27 (16%)	2	12
1	C	161/193 (83%)	137 (85%)	24 (15%)	3	15
1	E	158/193 (82%)	138 (87%)	20 (13%)	4	20
1	G	139/193 (72%)	115 (83%)	24 (17%)	2	10
2	B	162/182 (89%)	136 (84%)	26 (16%)	2	13
2	D	159/182 (87%)	128 (80%)	31 (20%)	1	8
2	F	162/182 (89%)	131 (81%)	31 (19%)	1	9
2	H	139/182 (76%)	120 (86%)	19 (14%)	3	18
All	All	1245/1500 (83%)	1043 (84%)	202 (16%)	2	12

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	LEU
1	A	11	LEU
1	A	12	VAL
1	A	18	LEU
1	A	35	GLN
1	A	43	LYS
1	A	48	VAL
1	A	63	GLU
1	A	64	VAL
1	A	68	PHE
1	A	74	ASN
1	A	78	THR
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	147	LEU
1	A	159	VAL
1	A	161	VAL
1	A	164	ASN
1	A	168	LEU
1	A	188	SER
1	A	198	LEU
1	A	218	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	7	SER
2	B	11	LEU
2	B	13	VAL
2	B	14	SER
2	B	21	LEU
2	B	28	SER
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	117	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	12	VAL
1	C	28	THR
1	C	33	ASP
1	C	35	GLN
1	C	45	LEU
1	C	46	GLU
1	C	78	THR
1	C	98	ARG
1	C	99	ARG
1	C	116	THR
1	C	117	LEU
1	C	125	THR
1	C	129	SER
1	C	147	LEU
1	C	151	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	159	VAL
1	C	168	LEU
1	C	179	LEU
1	C	187	LEU
1	C	190	VAL
1	C	192	THR
1	C	195	SER
1	C	214	THR
2	D	3	VAL
2	D	4	LEU
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	55	GLU
2	D	65	SER
2	D	69	THR
2	D	74	THR
2	D	75	ILE
2	D	97	THR
2	D	107	LYS
2	D	108	ARG
2	D	125	LEU
2	D	154	LEU
2	D	159	SER
2	D	161	GLU
2	D	163	VAL
2	D	166	GLN
2	D	172	THR
2	D	185	ASP
2	D	191	VAL
2	D	197	THR
2	D	203	SER
2	D	210	ASN
1	E	6	GLU
1	E	12	VAL
1	E	20	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	21	SER
1	E	35	GLN
1	E	37	VAL
1	E	51	ILE
1	E	68	PHE
1	E	81	LEU
1	E	82	GLN
1	E	87	ARG
1	E	110	ASP
1	E	116	THR
1	E	149	CYS
1	E	162	SER
1	E	169	THR
1	E	191	VAL
1	E	192	THR
1	E	206	ASN
1	E	214	THR
2	F	1	GLU
2	F	4	LEU
2	F	17	GLU
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	58	ILE
2	F	61	ARG
2	F	63	SER
2	F	65	SER
2	F	69	THR
2	F	75	ILE
2	F	78	LEU
2	F	85	THR
2	F	110	VAL
2	F	114	SER
2	F	135	LEU
2	F	136	LEU
2	F	154	LEU
2	F	163	VAL
2	F	164	THR
2	F	167	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	172	THR
2	F	177	SER
2	F	178	THR
2	F	179	LEU
2	F	182	SER
2	F	205	VAL
1	G	1	GLN
1	G	4	LEU
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	153	ASP
1	G	162	SER
1	G	165	SER
1	G	187	LEU
1	G	190	VAL
1	G	200	THR
1	G	206	ASN
1	G	213	ASN
1	G	217	ASP
1	G	220	VAL
2	H	13	VAL
2	H	17	GLU
2	H	21	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	133	VAL
2	H	147	GLN
2	H	172	THR
2	H	179	LEU
2	H	187	GLU
2	H	197	THR
2	H	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	77	ASN
1	A	173	HIS
1	A	180	GLN
1	A	206	ASN
2	B	6	GLN
2	B	37	GLN
2	B	38	GLN
2	B	137	ASN
2	B	158	ASN
2	B	189	HIS
2	B	198	HIS
2	B	199	GLN
1	C	35	GLN
1	C	77	ASN
1	C	173	HIS
1	C	206	ASN
2	D	124	GLN
2	D	137	ASN
2	D	158	ASN
2	D	160	GLN
1	E	39	GLN
1	E	173	HIS
1	E	209	HIS
2	F	6	GLN
2	F	38	GLN
2	F	42	GLN
2	F	155	GLN
2	F	198	HIS
1	G	74	ASN
1	G	206	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	124	GLN
2	H	147	GLN

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 oligosaccharides 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 ⓘ

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, 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	222/227 (97%)	0.06	2 (0%) 81 64	14, 47, 71, 84	0
1	C	223/227 (98%)	0.23	1 (0%) 88 79	35, 56, 68, 80	0
1	E	216/227 (95%)	0.16	2 (0%) 81 64	26, 53, 64, 74	0
1	G	220/227 (96%)	0.39	4 (1%) 67 48	51, 76, 88, 90	0
2	B	214/214 (100%)	-0.00	2 (0%) 81 64	22, 46, 71, 78	0
2	D	214/214 (100%)	-0.06	1 (0%) 87 76	17, 39, 63, 76	0
2	F	214/214 (100%)	0.05	2 (0%) 81 64	17, 41, 64, 70	0
2	H	214/214 (100%)	0.28	6 (2%) 55 35	37, 63, 85, 89	0
All	All	1737/1764 (98%)	0.14	20 (1%) 76 58	14, 53, 82, 90	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	112	TRP	3.6
1	E	2	VAL	3.4
2	H	214	CYS	2.8
2	D	179	LEU	2.8
1	A	147	LEU	2.7
2	B	68	GLY	2.6
1	G	97	ALA	2.6
2	F	73	LEU	2.6
1	G	136	CYS	2.6
2	H	8	PRO	2.3
1	G	216	VAL	2.3
2	F	91	TYR	2.2
2	H	186	TYR	2.2
2	B	135	LEU	2.2
1	C	223	LYS	2.2
1	A	203	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	60	ALA	2.2
2	H	93	ASP	2.1
2	H	62	PHE	2.1
1	E	159	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 oligosaccharides 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.