



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2024 – 10:05 AM EST

PDB ID : 8EB2
Title : Structure of HLA-A*02:01 in complex with NY-ESO-1 peptide and PA2.1 Fab
Authors : Jette, C.A.; West, A.P.
Deposited on : 2022-08-30
Resolution : 2.90 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
Xtrriage (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

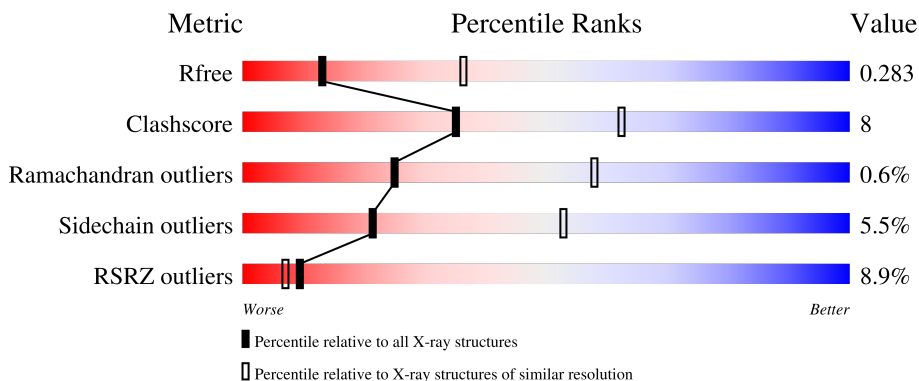
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	275	 77% 21%
1	D	275	 77% 23%
1	G	275	 79% 20%
2	B	100	 84% 16%
2	E	100	 7% 87% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	100	<p>5% 85% 13%</p>
3	C	9	<p>56% 44%</p>
3	F	9	<p>33% 56% 11%</p>
3	I	9	<p>11% 67% 22% 11%</p>
4	J	221	<p>2% 71% 22%</p>
4	K	221	<p>23% 75% 21%</p>
4	N	221	<p>38% 62% 31% 5%</p>
5	L	219	<p>78% 21%</p>
5	M	219	<p>5% 81% 16%</p>
5	O	219	<p>22% 78% 19%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19374 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 HLA-A*02:01 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	D	274	Total	C	N	O	S	0	0	0
			2237	1398	408	422	9			
1	G	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	H	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called NY-ESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	9	75	51	11	12	1	0	0	0

- Molecule 4 is a protein called PA2.1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	215	1628	1032	267	323	6	0	0	0
4	K	215	1628	1032	267	323	6	0	0	0
4	N	215	1628	1032	267	323	6	0	0	0

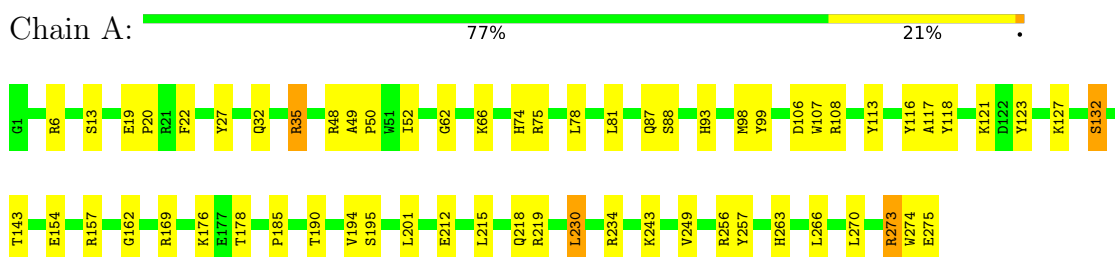
- Molecule 5 is a protein called PA2.1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	218	1683	1052	288	338	5	0	0	0
5	M	217	1671	1044	287	335	5	0	0	0
5	O	217	1673	1046	287	335	5	0	0	0

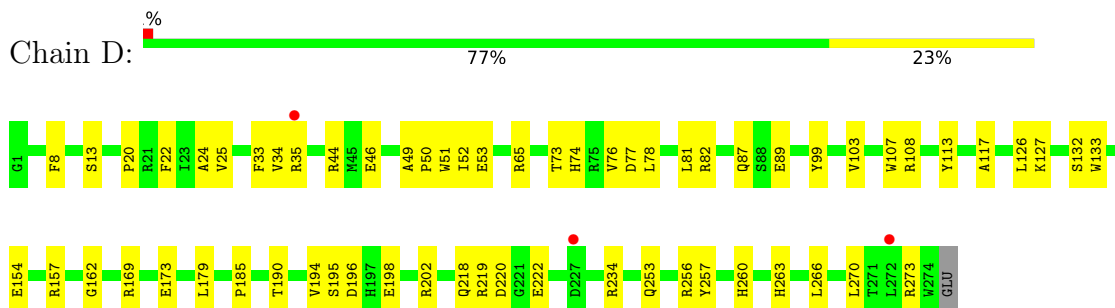
3 Residue-property plots [i](#)

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.

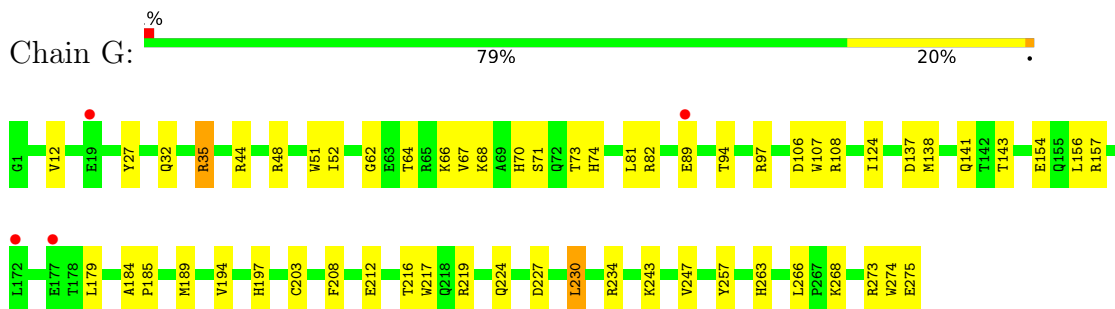
- Molecule 1: HLA-A*02:01 alpha chain



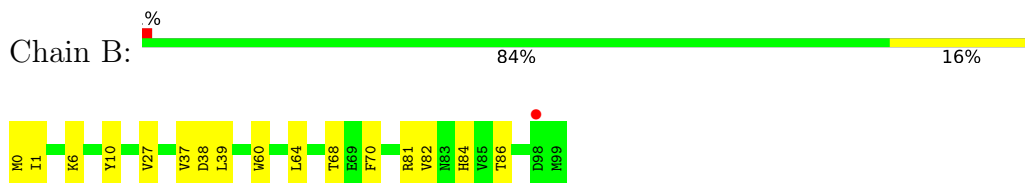
- Molecule 1: HLA-A*02:01 alpha chain



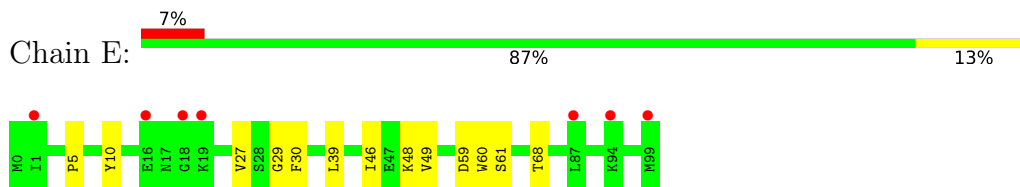
- Molecule 1: HLA-A*02:01 alpha chain



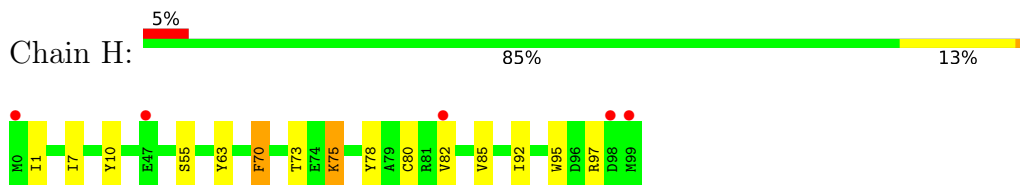
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



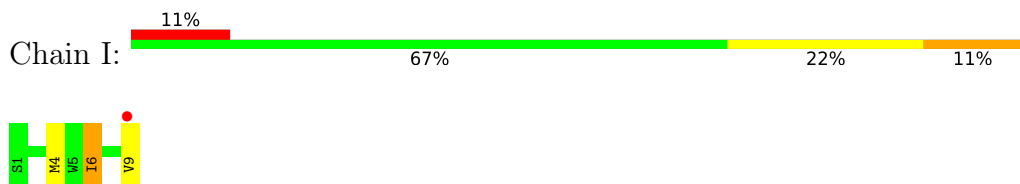
- Molecule 3: NY-ESO-1 peptide



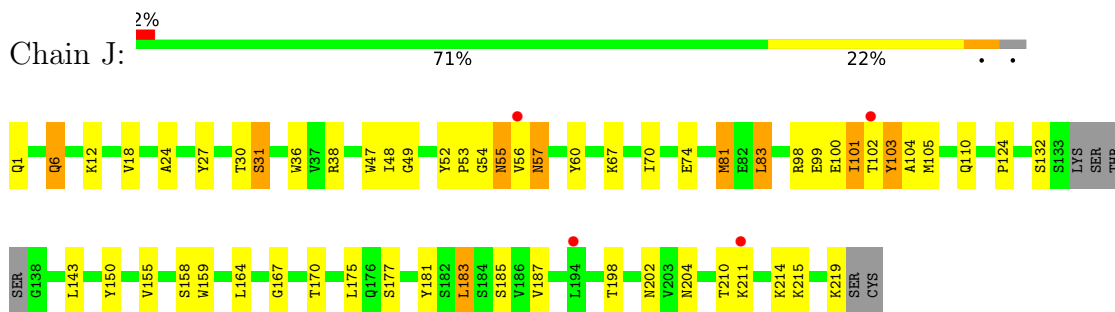
- Molecule 3: NY-ESO-1 peptide



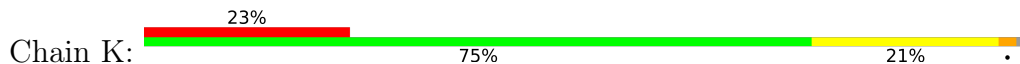
- Molecule 3: NY-ESO-1 peptide

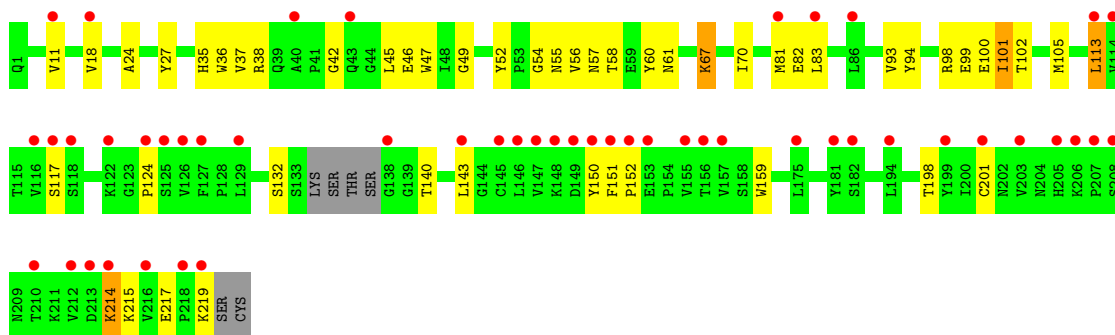


- Molecule 4: PA2.1 Fab Heavy Chain

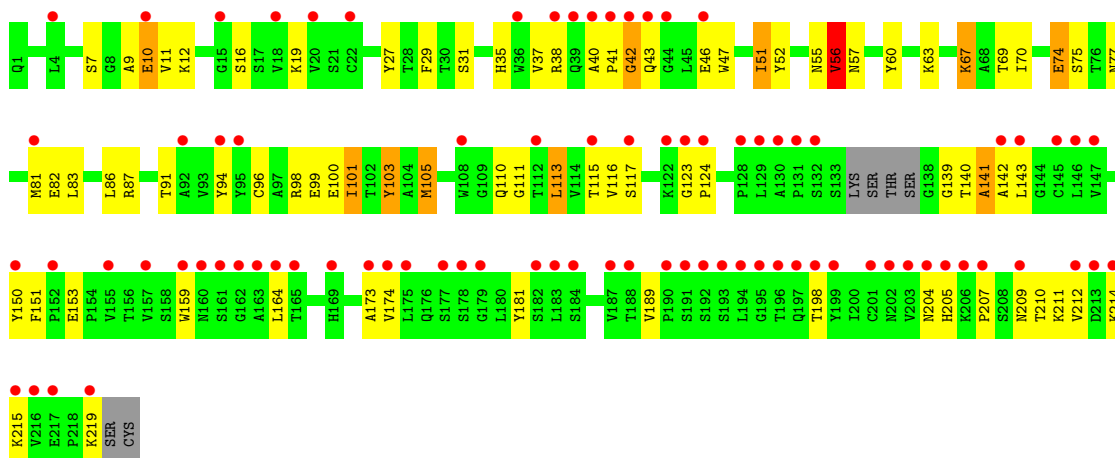


- Molecule 4: PA2.1 Fab Heavy Chain

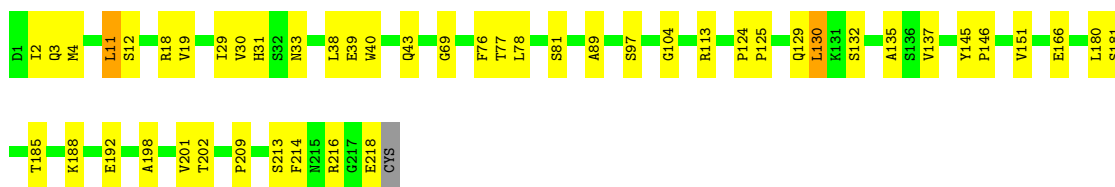




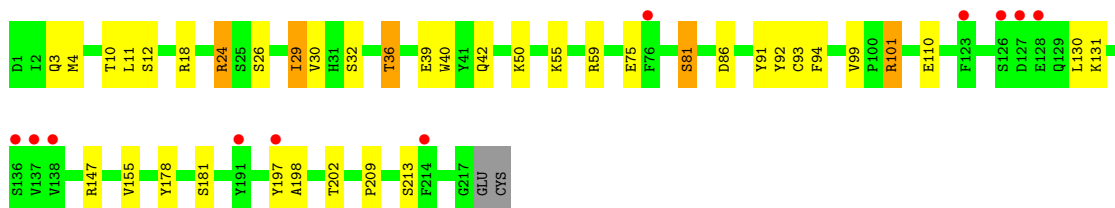
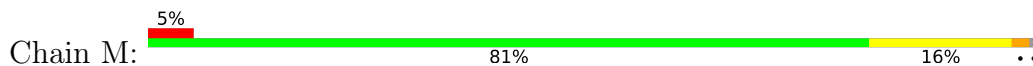
● Molecule 4: PA2.1 Fab Heavy Chain




● Molecule 5: PA2.1 Fab Light Chain

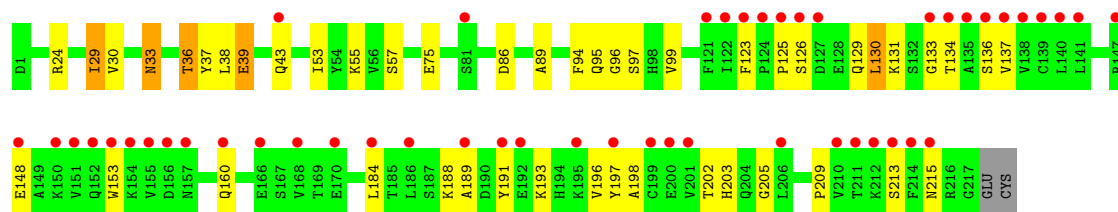


● Molecule 5: PA2.1 Fab Light Chain



● Molecule 5: PA2.1 Fab Light Chain

Chain O:  22% 78% 19% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.80Å 148.79Å 199.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 2.90 49.59 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.59-2.90) 83.9 (49.59-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.239 , 0.284 0.236 , 0.283	Depositor DCC
R_{free} test set	1999 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19374	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/2311	0.74	1/3137 (0.0%)
1	D	0.51	0/2302	0.70	1/3125 (0.0%)
1	G	0.48	0/2311	0.70	1/3137 (0.0%)
2	B	0.56	0/860	0.74	1/1162 (0.1%)
2	E	0.45	0/859	0.66	0/1162
2	H	0.43	0/859	0.67	0/1162
3	C	0.38	0/76	0.77	0/103
3	F	0.55	0/76	0.97	0/103
3	I	0.68	0/76	0.83	0/103
4	J	0.53	0/1669	0.71	0/2276
4	K	0.43	0/1669	0.65	0/2276
4	N	0.45	0/1669	0.66	0/2276
5	L	0.59	0/1720	0.78	2/2333 (0.1%)
5	M	0.47	0/1708	0.67	1/2317 (0.0%)
5	O	0.41	0/1710	0.68	0/2319
All	All	0.49	0/19875	0.70	7/26991 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	11	LEU	CB-CG-CD1	-6.24	100.40	111.00
2	B	64	LEU	CB-CG-CD1	-6.00	100.81	111.00
5	L	11	LEU	CA-CB-CG	5.50	127.95	115.30
1	G	156	LEU	CA-CB-CG	5.48	127.91	115.30
5	M	11	LEU	CA-CB-CG	5.14	127.11	115.30
1	D	77	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	230	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2246	0	2096	46	0
1	D	2237	0	2090	46	0
1	G	2246	0	2096	37	0
2	B	837	0	803	8	0
2	E	836	0	803	11	0
2	H	836	0	803	8	0
3	C	75	0	83	3	0
3	F	75	0	83	7	0
3	I	75	0	83	6	0
4	J	1628	0	1585	38	0
4	K	1628	0	1585	32	0
4	N	1628	0	1585	44	0
5	L	1683	0	1637	24	0
5	M	1671	0	1622	16	0
5	O	1673	0	1627	24	0
All	All	19374	0	18581	312	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 8.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:HIS:HA	3:I:6:ILE:HD11	1.50	0.94
1:A:35:ARG:HD2	1:A:48:ARG:HE	1.35	0.91
1:G:154:GLU:HG3	1:G:157:ARG:HH22	1.36	0.90
1:A:108:ARG:NH1	4:K:99:GLU:OE2	2.11	0.84
4:K:100:GLU:O	4:K:102:THR:N	2.11	0.84
1:G:230:LEU:HD21	1:G:243:LYS:HE3	1.60	0.82
1:A:127:LYS:HD3	1:A:132:SER:HB2	1.61	0.80
4:J:74:GLU:OE1	4:J:74:GLU:N	2.15	0.78
5:L:130:LEU:HD12	5:L:188:LYS:HG3	1.67	0.77
4:J:55:ASN:O	4:J:57:ASN:N	2.17	0.77
1:A:162:GLY:HA2	4:K:101:ILE:HD13	1.67	0.77
5:L:18:ARG:HE	5:L:81:SER:HB2	1.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:100:GLU:HG2	4:J:101:ILE:HD13	1.71	0.73
5:O:125:PRO:HD3	5:O:137:VAL:HG22	1.70	0.73
5:L:18:ARG:HG3	5:L:81:SER:HA	1.71	0.72
4:N:91:THR:HG23	4:N:115:THR:HA	1.70	0.72
1:A:169:ARG:HH12	4:K:101:ILE:HG22	1.55	0.69
1:A:87:GLN:OE1	1:A:93:HIS:NE2	2.26	0.69
4:N:29:PHE:HB2	4:N:77:ASN:HD22	1.58	0.69
4:K:124:PRO:HB3	4:K:150:TYR:HB3	1.74	0.69
1:D:162:GLY:HA2	4:J:101:ILE:HG13	1.74	0.68
1:G:108:ARG:HH12	4:N:99:GLU:CD	1.96	0.67
4:N:40:ALA:O	4:N:42:GLY:N	2.24	0.67
5:O:29:ILE:HG13	5:O:95:GLN:HB2	1.76	0.66
4:N:60:TYR:HE2	4:N:70:ILE:HG13	1.59	0.65
4:N:159:TRP:HB3	4:N:164:LEU:HD23	1.79	0.65
5:O:33:ASN:ND2	5:O:37:TYR:OH	2.29	0.65
4:N:55:ASN:C	4:N:57:ASN:H	2.01	0.63
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.80	0.63
4:J:55:ASN:C	4:J:57:ASN:H	2.02	0.63
5:O:30:VAL:HG22	5:O:36:THR:HB	1.79	0.63
2:H:7:ILE:HD12	2:H:82:VAL:HG21	1.80	0.63
4:J:36:TRP:CD2	4:J:81:MET:HG3	2.33	0.62
4:N:113:LEU:H	4:N:113:LEU:HD12	1.65	0.62
5:M:30:VAL:HG12	5:M:36:THR:HG23	1.80	0.62
1:A:6:ARG:HG2	1:A:98:MET:HE2	1.82	0.61
1:G:230:LEU:CD2	1:G:243:LYS:HE3	2.29	0.61
5:M:24:ARG:HH11	5:M:24:ARG:HB3	1.66	0.60
5:O:202:THR:HG22	5:O:209:PRO:HG3	1.83	0.60
5:L:198:ALA:HB2	5:L:213:SER:HB3	1.83	0.60
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.84	0.60
4:K:60:TYR:HE1	4:K:70:ILE:HG13	1.67	0.60
1:D:108:ARG:NH1	4:J:99:GLU:OE1	2.32	0.59
1:A:13:SER:HA	1:A:20:PRO:HB3	1.83	0.59
1:G:143:THR:HG21	3:I:9:VAL:HG22	1.85	0.59
4:K:198:THR:HG23	4:K:215:LYS:HE3	1.84	0.58
1:D:107:TRP:O	1:D:169:ARG:NH2	2.36	0.58
5:L:145:TYR:CD1	5:L:146:PRO:HA	2.39	0.58
4:J:159:TRP:HB3	4:J:164:LEU:HD23	1.84	0.58
4:J:38:ARG:HB3	4:J:48:ILE:HD11	1.84	0.58
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.86	0.58
1:A:176:LYS:NZ	4:K:54:GLY:O	2.23	0.58
4:N:37:VAL:HG22	4:N:47:TRP:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HG3	1:A:157:ARG:HH22	1.70	0.57
1:D:13:SER:HA	1:D:20:PRO:HB3	1.86	0.57
4:N:51:ILE:HD11	4:N:56:VAL:HA	1.87	0.56
1:G:189:MET:HG2	1:G:274:TRP:CZ2	2.40	0.56
1:G:154:GLU:HG3	1:G:157:ARG:NH2	2.15	0.56
4:N:100:GLU:OE1	4:N:101:ILE:HG12	2.05	0.56
4:N:67:LYS:O	4:N:83:LEU:HD12	2.05	0.56
5:O:33:ASN:OD1	5:O:33:ASN:N	2.26	0.56
1:A:22:PHE:HE1	1:A:74:HIS:HD1	1.54	0.56
5:L:113:ARG:HG3	5:L:145:TYR:CD2	2.41	0.55
1:A:154:GLU:HG3	1:A:157:ARG:NH2	2.21	0.55
1:A:143:THR:HG21	3:C:9:VAL:HG22	1.87	0.55
4:N:19:LYS:HA	4:N:81:MET:O	2.06	0.55
4:N:204:ASN:CG	4:N:211:LYS:HE2	2.26	0.55
1:A:185:PRO:HD3	1:A:263:HIS:ND1	2.22	0.55
5:L:43:GLN:O	5:L:89:ALA:HB1	2.07	0.55
4:K:36:TRP:CE2	4:K:81:MET:HB2	2.42	0.55
5:O:198:ALA:HB2	5:O:213:SER:HB3	1.89	0.55
1:A:274:TRP:HZ3	3:F:4:MET:HG2	1.72	0.54
5:L:188:LYS:O	5:L:192:GLU:HG2	2.07	0.54
5:L:29:ILE:HD11	5:L:76:PHE:CE2	2.43	0.54
1:D:169:ARG:HH12	4:J:101:ILE:HG22	1.73	0.53
4:J:54:GLY:O	4:J:55:ASN:HB2	2.08	0.53
1:G:108:ARG:NH1	4:N:99:GLU:OE2	2.33	0.53
1:D:219:ARG:O	1:D:222:GLU:HB3	2.09	0.53
2:H:75:LYS:HD3	2:H:75:LYS:H	1.74	0.53
4:N:74:GLU:HG3	4:N:75:SER:N	2.22	0.53
5:L:125:PRO:HD3	5:L:137:VAL:HG22	1.91	0.52
5:M:3:GLN:HB2	5:M:26:SER:HB3	1.90	0.52
1:D:22:PHE:HE1	1:D:74:HIS:HD1	1.57	0.52
5:L:166:GLU:HB2	5:L:180:LEU:HD21	1.92	0.52
5:M:29:ILE:O	5:M:36:THR:HG22	2.09	0.52
1:G:82:ARG:NE	1:G:89:GLU:HG2	2.24	0.52
1:G:219:ARG:HG3	1:G:257:TYR:CZ	2.45	0.52
1:G:66:LYS:HD3	3:I:4:MET:HA	1.91	0.52
4:K:11:VAL:HG21	4:K:152:PRO:HG3	1.91	0.52
1:G:81:LEU:HD21	3:I:9:VAL:HG11	1.92	0.52
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.44	0.52
4:J:12:LYS:HE3	4:J:18:VAL:HG23	1.91	0.52
1:D:219:ARG:HG3	1:D:257:TYR:CZ	2.44	0.51
4:J:198:THR:HG23	4:J:215:LYS:HE3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.51
4:J:31:SER:HA	4:J:52:TYR:OH	2.10	0.51
5:L:192:GLU:O	5:L:216:ARG:NH2	2.43	0.51
4:K:55:ASN:OD1	4:K:57:ASN:HB2	2.11	0.51
5:L:202:THR:HG22	5:L:209:PRO:HG3	1.92	0.51
4:N:141:ALA:HB3	4:N:189:VAL:O	2.11	0.51
1:A:274:TRP:CZ3	3:F:4:MET:HG2	2.46	0.50
1:G:62:GLY:O	1:G:66:LYS:HG3	2.10	0.50
4:K:67:LYS:O	4:K:83:LEU:HD12	2.11	0.50
1:D:195:SER:HB3	1:D:198:GLU:HB2	1.92	0.50
4:J:6:GLN:O	4:J:110:GLN:NE2	2.44	0.50
4:K:60:TYR:CE1	4:K:70:ILE:HG13	2.46	0.50
4:N:142:ALA:HB1	5:O:123:PHE:HZ	1.76	0.50
4:J:24:ALA:HB1	4:J:27:TYR:CE1	2.46	0.50
1:D:82:ARG:CZ	1:D:89:GLU:HG2	2.42	0.50
4:J:36:TRP:CG	4:J:81:MET:HG3	2.47	0.50
1:A:27:TYR:CE2	1:A:32:GLN:HB2	2.47	0.50
3:F:4:MET:HB3	3:F:5:TRP:HE3	1.77	0.49
1:D:50:PRO:O	1:D:53:GLU:HB2	2.12	0.49
2:H:55:SER:HB3	2:H:63:TYR:CZ	2.47	0.49
5:M:42:GLN:HG3	5:M:91:TYR:CE1	2.47	0.49
4:N:55:ASN:O	4:N:57:ASN:N	2.46	0.49
4:N:142:ALA:CB	5:O:123:PHE:HZ	2.25	0.49
3:I:6:ILE:H	3:I:6:ILE:HD12	1.76	0.49
1:D:234:ARG:HD2	2:E:10:TYR:CE1	2.48	0.49
4:J:158:SER:OG	4:J:202:ASN:HB2	2.13	0.49
4:K:159:TRP:CH2	4:K:201:CYS:HB3	2.48	0.49
2:B:0:MET:HG2	2:B:1:ILE:H	1.78	0.49
1:A:195:SER:O	1:D:76:VAL:HG11	2.12	0.48
4:K:159:TRP:CZ3	4:K:201:CYS:HB3	2.47	0.48
1:G:74:HIS:CD2	1:G:97:ARG:HH21	2.31	0.48
5:L:180:LEU:HD23	5:L:181:SER:N	2.28	0.48
4:J:60:TYR:HE1	4:J:70:ILE:HG13	1.79	0.48
5:M:202:THR:HG22	5:M:209:PRO:HG3	1.95	0.48
1:D:82:ARG:HD2	1:D:89:GLU:HA	1.95	0.48
5:L:166:GLU:HA	5:L:181:SER:O	2.14	0.48
5:L:31:HIS:HB3	5:L:33:ASN:OD1	2.14	0.48
4:N:124:PRO:HB3	4:N:150:TYR:HB3	1.95	0.47
1:D:169:ARG:NH1	4:J:101:ILE:HG22	2.30	0.47
1:G:227:ASP:O	1:G:247:VAL:HG23	2.15	0.47
2:E:27:VAL:HG23	2:E:30:PHE:HE2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:175:LEU:HD13	4:J:181:TYR:CE1	2.49	0.47
4:K:58:THR:HG1	4:K:60:TYR:HE2	1.62	0.47
5:L:125:PRO:HG3	5:L:135:ALA:HB1	1.96	0.47
4:K:24:ALA:HB1	4:K:27:TYR:HE1	1.79	0.47
4:N:16:SER:O	4:N:86:LEU:HG	2.15	0.47
4:N:37:VAL:HG13	4:N:46:GLU:O	2.15	0.47
1:A:194:VAL:HG13	1:A:195:SER:H	1.78	0.47
1:A:35:ARG:HG2	1:A:48:ARG:CG	2.45	0.47
4:N:12:LYS:HE2	4:N:12:LYS:HA	1.95	0.47
5:O:43:GLN:O	5:O:89:ALA:HB1	2.14	0.47
5:L:69:GLY:HA2	5:L:77:THR:O	2.15	0.46
1:A:116:TYR:HD2	1:A:123:TYR:HD2	1.64	0.46
4:N:174:VAL:O	4:N:181:TYR:HA	2.15	0.46
1:G:35:ARG:HG2	1:G:48:ARG:HE	1.80	0.46
1:G:234:ARG:HD2	2:H:10:TYR:CE1	2.51	0.46
4:J:204:ASN:HD22	4:J:211:LYS:HG2	1.79	0.46
4:K:47:TRP:CE3	4:K:61:ASN:HB2	2.51	0.46
1:D:49:ALA:O	1:D:52:ILE:HG22	2.16	0.46
4:N:55:ASN:C	4:N:57:ASN:N	2.69	0.46
2:B:38:ASP:HB2	2:B:81:ARG:HB3	1.98	0.46
4:N:35:HIS:O	4:N:96:CYS:HA	2.15	0.46
4:J:155:VAL:HG22	4:J:183:LEU:HD21	1.97	0.46
4:J:83:LEU:HA	4:J:83:LEU:HD12	1.68	0.46
4:J:124:PRO:HD2	4:J:210:THR:HG21	1.98	0.46
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.51	0.46
1:G:107:TRP:CE3	4:N:52:TYR:CE2	3.03	0.46
1:A:35:ARG:HG2	1:A:48:ARG:HG3	1.98	0.46
1:G:27:TYR:CE2	1:G:32:GLN:HB2	2.51	0.46
5:O:196:VAL:HG22	5:O:215:ASN:OD1	2.16	0.45
5:O:203:HIS:CE1	5:O:205:GLY:H	2.35	0.45
1:A:52:ILE:HG13	1:A:52:ILE:O	2.17	0.45
1:G:212:GLU:O	1:G:263:HIS:HD2	1.99	0.45
5:M:24:ARG:HB3	5:M:24:ARG:NH1	2.31	0.45
1:A:219:ARG:HD3	1:A:256:ARG:CZ	2.47	0.45
3:C:8:GLN:CD	3:C:8:GLN:H	2.18	0.45
1:D:8:PHE:O	1:D:24:ALA:HA	2.16	0.45
2:B:6:LYS:O	2:B:27:VAL:HA	2.17	0.45
1:A:106:ASP:CG	1:A:108:ARG:HG3	2.37	0.45
1:A:201:LEU:HD12	1:A:249:VAL:HG11	1.99	0.45
5:M:147:ARG:HB2	5:M:178:TYR:CE2	2.51	0.45
5:O:191:TYR:HA	5:O:197:TYR:OH	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:94:PHE:CZ	5:M:101:ARG:HB2	2.52	0.45
5:M:198:ALA:HB2	5:M:213:SER:HB3	1.99	0.45
4:N:11:VAL:HG21	4:N:151:PHE:CZ	2.52	0.45
1:G:219:ARG:HB2	1:G:224:GLN:HG3	1.99	0.45
5:O:153:TRP:HB2	5:O:160:GLN:HB2	1.98	0.45
4:N:210:THR:HG22	4:N:212:VAL:HG23	1.99	0.45
4:J:204:ASN:ND2	4:J:211:LYS:HG2	2.32	0.44
4:K:24:ALA:HB1	4:K:27:TYR:CE1	2.52	0.44
4:N:69:THR:N	4:N:82:GLU:O	2.42	0.44
1:A:107:TRP:CE3	4:K:52:TYR:CZ	3.05	0.44
1:D:266:LEU:HD13	1:D:270:LEU:HG	1.99	0.44
2:E:29:GLY:HA2	2:E:61:SER:CB	2.47	0.44
1:D:196:ASP:OD1	1:D:196:ASP:N	2.45	0.44
1:G:52:ILE:HG13	1:G:52:ILE:O	2.17	0.44
4:N:98:ARG:HG2	4:N:99:GLU:N	2.32	0.44
5:O:129:GLN:HG2	5:O:134:THR:O	2.17	0.44
1:G:137:ASP:O	1:G:141:GLN:HG2	2.17	0.44
4:J:170:THR:HG23	4:J:185:SER:HB2	2.00	0.44
5:L:40:TRP:CE2	5:L:78:LEU:HB2	2.52	0.44
4:K:37:VAL:HG13	4:K:46:GLU:O	2.17	0.44
5:M:18:ARG:HG3	5:M:81:SER:HA	1.99	0.44
4:N:209:ASN:OD1	4:N:211:LYS:HE3	2.17	0.44
1:D:99:TYR:CE2	3:F:3:LEU:HD12	2.52	0.44
5:L:124:PRO:HB3	5:L:214:PHE:CE1	2.53	0.44
5:M:40:TRP:CZ3	5:M:93:CYS:HB3	2.53	0.44
1:D:99:TYR:CZ	3:F:3:LEU:HD12	2.53	0.44
1:G:73:THR:HB	3:I:6:ILE:HD13	2.00	0.44
1:G:185:PRO:HA	1:G:208:PHE:HB3	1.99	0.44
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.53	0.44
1:D:103:VAL:HA	1:D:108:ARG:O	2.18	0.43
2:H:95:TRP:CH2	2:H:97:ARG:HG2	2.52	0.43
4:K:38:ARG:HB2	4:K:94:TYR:CE1	2.53	0.43
4:K:117:SER:HB3	4:K:151:PHE:CZ	2.52	0.43
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.53	0.43
2:E:5:PRO:HB3	2:E:30:PHE:HB3	1.99	0.43
2:H:73:THR:O	2:H:97:ARG:NH2	2.52	0.43
1:D:73:THR:HG23	3:F:8:GLN:HG3	2.00	0.43
1:G:68:LYS:O	1:G:71:SER:HB3	2.18	0.43
4:J:99:GLU:HA	4:J:104:ALA:O	2.18	0.43
5:O:39:GLU:HG3	5:O:94:PHE:HB3	2.00	0.43
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:12:SER:HB3	5:M:110:GLU:OE2	2.19	0.43
2:E:39:LEU:HD23	2:E:68:THR:HG22	2.01	0.43
5:O:126:SER:O	5:O:130:LEU:HD22	2.19	0.43
4:J:47:TRP:CZ2	4:J:49:GLY:HA2	2.54	0.43
4:J:103:TYR:CD1	4:J:103:TYR:N	2.85	0.43
1:D:87:GLN:HE21	1:D:87:GLN:HB2	1.67	0.43
4:J:30:THR:HA	4:J:53:PRO:HB2	2.01	0.43
1:A:118:TYR:O	1:A:121:LYS:HG2	2.19	0.43
1:D:13:SER:HB3	1:D:78:LEU:HD13	2.01	0.43
5:L:129:GLN:O	5:L:132:SER:OG	2.26	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.42
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.87	0.42
1:D:8:PHE:HB2	1:D:25:VAL:HG23	2.01	0.42
1:D:126:LEU:HD13	1:D:133:TRP:CH2	2.54	0.42
1:D:195:SER:OG	1:D:196:ASP:OD1	2.37	0.42
4:N:205:HIS:CD2	4:N:207:PRO:HD2	2.54	0.42
1:D:218:GLN:OE1	1:D:260:HIS:NE2	2.52	0.42
2:E:46:ILE:HG22	2:E:48:LYS:H	1.84	0.42
4:K:214:LYS:HB2	4:K:214:LYS:NZ	2.33	0.42
1:A:169:ARG:NH1	4:K:101:ILE:HG22	2.28	0.42
2:E:29:GLY:HA2	2:E:61:SER:HB2	2.00	0.42
2:E:59:ASP:OD1	2:E:59:ASP:N	2.53	0.42
4:J:36:TRP:CE2	4:J:81:MET:HG3	2.54	0.42
5:L:151:VAL:HG22	5:L:201:VAL:HG22	2.01	0.42
4:K:27:TYR:CE2	4:K:98:ARG:HD2	2.55	0.42
1:G:108:ARG:NH1	4:N:99:GLU:OE1	2.53	0.42
5:L:11:LEU:HD11	5:L:19:VAL:HG13	2.00	0.42
5:O:133:GLY:HA2	5:O:188:LYS:HB2	2.02	0.42
1:D:52:ILE:O	1:D:52:ILE:HG13	2.20	0.42
1:D:194:VAL:HG13	1:D:195:SER:H	1.85	0.42
1:D:253:GLN:HB3	1:D:256:ARG:HD3	2.02	0.42
2:H:80:CYS:O	2:H:92:ILE:HA	2.19	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.42
2:E:39:LEU:HB2	2:E:49:VAL:HG21	2.02	0.42
5:M:18:ARG:HE	5:M:81:SER:HB3	1.84	0.42
4:N:124:PRO:HD2	4:N:210:THR:HB	2.00	0.42
1:D:44:ARG:O	1:D:46:GLU:HG3	2.19	0.42
1:D:73:THR:HB	3:F:6:ILE:HD11	2.02	0.42
5:O:136:SER:HA	5:O:184:LEU:O	2.20	0.42
4:J:98:ARG:HG2	4:J:99:GLU:N	2.35	0.42
4:J:124:PRO:HB3	4:J:150:TYR:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:94:TYR:O	4:N:111:GLY:HA2	2.20	0.42
4:N:123:GLY:HA3	4:N:210:THR:OG1	2.20	0.42
4:N:153:GLU:OE2	4:N:173:ALA:HB3	2.19	0.42
5:O:55:LYS:O	5:O:57:SER:N	2.42	0.42
1:G:51:TRP:CZ2	1:G:179:LEU:HD11	2.55	0.42
1:A:190:THR:HG22	1:D:65:ARG:HD2	2.01	0.41
4:K:98:ARG:HG2	4:K:99:GLU:N	2.35	0.41
5:M:155:VAL:HG22	5:M:197:TYR:CD1	2.54	0.41
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.20	0.41
2:E:29:GLY:HA2	2:E:61:SER:OG	2.21	0.41
4:K:45:LEU:HD12	5:M:92:TYR:CD2	2.55	0.41
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.85	0.41
1:G:184:ALA:HB1	1:G:266:LEU:HD23	2.03	0.41
4:K:18:VAL:O	4:K:82:GLU:HA	2.21	0.41
4:N:198:THR:HG23	4:N:215:LYS:HE3	2.02	0.41
4:J:167:GLY:O	4:J:187:VAL:HA	2.20	0.41
5:L:4:MET:HB2	5:L:104:GLY:HA2	2.03	0.41
5:O:39:GLU:HA	5:O:53:ILE:O	2.21	0.41
1:A:19:GLU:HG2	1:A:75:ARG:NH2	2.36	0.41
1:A:107:TRP:HE3	4:K:52:TYR:HH	1.65	0.41
1:D:127:LYS:HD3	1:D:132:SER:OG	2.21	0.41
1:D:185:PRO:HD3	1:D:263:HIS:ND1	2.35	0.41
5:O:39:GLU:HG3	5:O:94:PHE:HD2	1.86	0.41
1:A:266:LEU:HD13	1:A:270:LEU:HG	2.02	0.41
4:N:86:LEU:HB3	4:N:116:VAL:HG11	2.02	0.41
1:A:99:TYR:CE2	3:C:3:LEU:HD12	2.56	0.41
1:A:116:TYR:HD2	1:A:123:TYR:CD2	2.39	0.41
1:D:107:TRP:CD1	1:D:107:TRP:N	2.86	0.41
1:D:220:ASP:OD1	1:D:256:ARG:HB3	2.21	0.41
1:G:185:PRO:HD3	1:G:263:HIS:ND1	2.36	0.41
1:A:273:ARG:HE	1:A:273:ARG:HB3	1.51	0.41
1:G:12:VAL:HG22	1:G:94:THR:HG23	2.02	0.41
1:G:44:ARG:HD2	1:G:64:THR:HG21	2.02	0.41
2:H:70:PHE:HD2	2:H:78:TYR:CZ	2.39	0.41
5:O:189:ALA:O	5:O:193:LYS:HG3	2.21	0.41
4:N:10:GLU:HB2	4:N:11:VAL:H	1.56	0.40
1:A:62:GLY:O	1:A:66:LYS:HG3	2.20	0.40
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.55	0.40
1:D:154:GLU:HG3	1:D:157:ARG:NH2	2.36	0.40
1:A:218:GLN:O	1:A:257:TYR:HA	2.21	0.40
1:D:81:LEU:HD23	1:D:81:LEU:HA	1.82	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:GLU:HG3	1:D:157:ARG:HH22	1.85	0.40
1:G:106:ASP:CG	1:G:108:ARG:HG3	2.41	0.40
4:K:93:VAL:HG22	4:K:113:LEU:HG	2.03	0.40
4:J:103:TYR:N	4:J:103:TYR:HD1	2.20	0.40
4:K:47:TRP:CZ2	4:K:49:GLY:HA2	2.57	0.40
4:N:98:ARG:O	4:N:105:MET:HA	2.21	0.40
5:O:148:GLU:O	5:O:203:HIS:HD2	2.04	0.40
1:A:212:GLU:O	1:A:263:HIS:HD2	2.03	0.40
1:G:64:THR:O	1:G:67:VAL:HG12	2.22	0.40
1:G:138:MET:O	1:G:141:GLN:HB2	2.21	0.40
4:J:24:ALA:HB1	4:J:27:TYR:HE1	1.86	0.40
4:J:55:ASN:C	4:J:57:ASN:N	2.66	0.40
4:N:27:TYR:CE2	4:N:98:ARG:HD2	2.56	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	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
1	D	272/275 (99%)	261 (96%)	11 (4%)	0	100	100
1	G	273/275 (99%)	260 (95%)	13 (5%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	H	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	7 (100%)	0	0	100	100
4	J	211/221 (96%)	197 (93%)	12 (6%)	2 (1%)	17	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	211/221 (96%)	193 (92%)	14 (7%)	4 (2%)	8	28
4	N	211/221 (96%)	192 (91%)	11 (5%)	8 (4%)	3	13
5	L	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
5	M	215/219 (98%)	204 (95%)	11 (5%)	0	100	100
5	O	215/219 (98%)	204 (95%)	10 (5%)	1 (0%)	29	61
All	All	2412/2472 (98%)	2284 (95%)	113 (5%)	15 (1%)	25	58

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	55	ASN
4	J	56	VAL
4	K	101	ILE
4	N	56	VAL
4	N	103	TYR
4	K	42	GLY
4	N	141	ALA
4	K	132	SER
4	N	9	ALA
4	N	139	GLY
4	N	31	SER
4	N	41	PRO
4	N	42	GLY
5	O	96	GLY
4	K	56	VAL

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	231/231 (100%)	223 (96%)	8 (4%)	36	70
1	D	230/231 (100%)	226 (98%)	4 (2%)	60	86
1	G	231/231 (100%)	222 (96%)	9 (4%)	32	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	95/95 (100%)	94 (99%)	1 (1%)	73 92
2	E	95/95 (100%)	95 (100%)	0	100 100
2	H	95/95 (100%)	91 (96%)	4 (4%)	30 63
3	C	9/9 (100%)	8 (89%)	1 (11%)	6 19
3	F	9/9 (100%)	7 (78%)	2 (22%)	1 3
3	I	9/9 (100%)	8 (89%)	1 (11%)	6 19
4	J	182/188 (97%)	165 (91%)	17 (9%)	9 27
4	K	182/188 (97%)	173 (95%)	9 (5%)	25 57
4	N	182/188 (97%)	162 (89%)	20 (11%)	6 19
5	L	193/194 (100%)	183 (95%)	10 (5%)	23 55
5	M	191/194 (98%)	173 (91%)	18 (9%)	8 26
5	O	192/194 (99%)	180 (94%)	12 (6%)	18 46
All	All	2126/2151 (99%)	2010 (94%)	116 (6%)	21 53

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	50	PRO
1	A	88	SER
1	A	113	TYR
1	A	132	SER
1	A	178	THR
1	A	273	ARG
1	A	275	GLU
2	B	70	PHE
3	C	4	MET
1	D	35	ARG
1	D	113	TYR
1	D	173	GLU
1	D	273	ARG
3	F	8	GLN
3	F	9	VAL
1	G	35	ARG
1	G	124	ILE
1	G	194	VAL
1	G	197	HIS
1	G	216	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	230	LEU
1	G	268	LYS
1	G	273	ARG
1	G	275	GLU
2	H	1	ILE
2	H	70	PHE
2	H	75	LYS
2	H	85	VAL
3	I	6	ILE
4	J	1	GLN
4	J	6	GLN
4	J	31	SER
4	J	57	ASN
4	J	67	LYS
4	J	81	MET
4	J	83	LEU
4	J	101	ILE
4	J	102	THR
4	J	103	TYR
4	J	105	MET
4	J	132	SER
4	J	143	LEU
4	J	177	SER
4	J	183	LEU
4	J	214	LYS
4	J	219	LYS
5	L	2	ILE
5	L	3	GLN
5	L	12	SER
5	L	30	VAL
5	L	38	LEU
5	L	39	GLU
5	L	97	SER
5	L	130	LEU
5	L	185	THR
5	L	218	GLU
4	K	35	HIS
4	K	67	LYS
4	K	105	MET
4	K	113	LEU
4	K	140	THR
4	K	143	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	214	LYS
4	K	217	GLU
4	K	219	LYS
5	M	4	MET
5	M	10	THR
5	M	24	ARG
5	M	29	ILE
5	M	32	SER
5	M	36	THR
5	M	39	GLU
5	M	50	LYS
5	M	55	LYS
5	M	59	ARG
5	M	75	GLU
5	M	81	SER
5	M	86	ASP
5	M	99	VAL
5	M	101	ARG
5	M	130	LEU
5	M	131	LYS
5	M	181	SER
4	N	7	SER
4	N	10	GLU
4	N	38	ARG
4	N	43	GLN
4	N	51	ILE
4	N	56	VAL
4	N	63	LYS
4	N	67	LYS
4	N	74	GLU
4	N	87	ARG
4	N	101	ILE
4	N	103	TYR
4	N	105	MET
4	N	110	GLN
4	N	113	LEU
4	N	117	SER
4	N	140	THR
4	N	143	LEU
4	N	214	LYS
4	N	219	LYS
5	O	24	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	O	29	ILE
5	O	33	ASN
5	O	36	THR
5	O	38	LEU
5	O	39	GLU
5	O	75	GLU
5	O	86	ASP
5	O	97	SER
5	O	99	VAL
5	O	130	LEU
5	O	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	87	GLN
1	D	145	HIS
4	J	204	ASN
5	L	35	ASN
4	K	43	GLN
4	N	77	ASN
4	N	110	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/275 (100%)	0.08	0 100 100	46, 64, 87, 123	0
1	D	274/275 (99%)	0.18	3 (1%) 80 80	45, 66, 163, 202	0
1	G	275/275 (100%)	0.37	4 (1%) 73 73	50, 83, 116, 169	0
2	B	100/100 (100%)	0.27	1 (1%) 82 82	42, 58, 92, 125	0
2	E	100/100 (100%)	0.51	7 (7%) 16 12	54, 93, 139, 158	0
2	H	100/100 (100%)	0.46	5 (5%) 28 25	61, 82, 120, 132	0
3	C	9/9 (100%)	0.82	0 100 100	57, 61, 72, 75	0
3	F	9/9 (100%)	0.33	0 100 100	46, 51, 58, 60	0
3	I	9/9 (100%)	1.11	1 (11%) 5 4	73, 88, 97, 100	0
4	J	215/221 (97%)	0.27	4 (1%) 66 65	46, 68, 106, 127	0
4	K	215/221 (97%)	1.07	50 (23%) 0 0	62, 107, 153, 183	0
4	N	215/221 (97%)	2.06	84 (39%) 0 0	80, 167, 239, 299	0
5	L	218/219 (99%)	0.01	0 100 100	42, 55, 82, 110	0
5	M	217/219 (99%)	0.32	11 (5%) 28 24	61, 80, 130, 147	0
5	O	217/219 (99%)	1.20	49 (22%) 0 0	74, 130, 192, 239	0
All	All	2448/2472 (99%)	0.56	219 (8%) 9 7	42, 79, 176, 299	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	194	LEU	12.9
4	N	212	VAL	12.4
4	N	155	VAL	11.3
4	N	203	VAL	10.7
4	N	214	LYS	10.1
4	N	143	LEU	7.5
4	N	199	TYR	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	215	LYS	6.9
4	N	216	VAL	6.8
5	O	122	ILE	6.8
4	N	201	CYS	6.7
5	O	199	CYS	6.7
5	O	214	PHE	6.4
4	K	212	VAL	6.3
5	O	140	LEU	6.3
4	N	38	ARG	6.3
4	N	43	GLN	6.1
4	N	112	THR	6.0
4	N	159	TRP	5.9
2	H	99	MET	5.8
4	N	217	GLU	5.6
4	N	206	LYS	5.5
4	N	152	PRO	5.5
4	N	187	VAL	5.2
4	N	193	SER	5.2
4	N	146	LEU	5.2
4	N	130	ALA	5.1
4	N	131	PRO	5.0
4	N	163	ALA	4.8
4	N	145	CYS	4.8
4	N	4	LEU	4.8
4	N	44	GLY	4.7
5	O	210	VAL	4.7
4	K	124	PRO	4.7
5	O	166	GLU	4.6
4	K	214	LYS	4.6
5	O	211	THR	4.6
5	O	123	PHE	4.6
4	N	204	ASN	4.5
4	N	15	GLY	4.5
4	N	115	THR	4.5
4	N	129	LEU	4.4
5	O	125	PRO	4.3
5	O	197	TYR	4.3
5	O	141	LEU	4.3
4	N	161	SER	4.3
4	N	162	GLY	4.3
5	M	127	ASP	4.2
4	N	147	VAL	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	157	VAL	4.2
4	K	155	VAL	4.1
4	K	203	VAL	4.1
4	N	198	THR	4.1
5	M	136	SER	3.9
4	N	191	SER	3.9
4	N	213	ASP	3.9
4	K	113	LEU	3.9
4	N	219	LYS	3.8
5	O	151	VAL	3.7
5	O	153	TRP	3.7
4	N	20	VAL	3.7
2	E	1	ILE	3.7
5	O	139	CYS	3.6
4	K	147	VAL	3.6
4	N	183	LEU	3.6
5	O	137	VAL	3.6
5	O	192	GLU	3.6
4	K	125	SER	3.6
4	N	195	GLY	3.6
4	N	81	MET	3.6
4	K	210	THR	3.6
4	N	174	VAL	3.6
4	K	127	PHE	3.5
4	N	190	PRO	3.5
4	N	128	PRO	3.5
5	O	127	ASP	3.4
4	K	146	LEU	3.4
5	O	157	ASN	3.4
4	K	151	PHE	3.3
4	K	216	VAL	3.3
4	N	188	THR	3.3
4	K	122	LYS	3.3
2	E	19	LYS	3.3
4	N	124	PRO	3.3
4	N	40	ALA	3.2
5	M	137	VAL	3.2
4	N	207	PRO	3.2
4	K	126	VAL	3.2
5	O	155	VAL	3.2
4	K	157	VAL	3.2
2	E	16	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	182	SER	3.1
4	N	46	GLU	3.1
5	O	135	ALA	3.1
4	N	132	SER	3.1
4	K	129	LEU	3.1
2	E	18	GLY	3.1
4	K	207	PRO	3.1
4	K	152	PRO	3.0
4	K	117	SER	3.0
4	N	173	ALA	3.0
5	M	138	VAL	3.0
4	K	40	ALA	3.0
5	O	201	VAL	3.0
4	N	184	SER	2.9
5	O	81	SER	2.9
4	K	194	LEU	2.9
4	K	218	PRO	2.9
4	K	118	SER	2.9
5	O	124	PRO	2.9
5	O	126	SER	2.9
5	O	138	VAL	2.9
4	K	143	LEU	2.9
4	N	142	ALA	2.9
1	G	19	GLU	2.9
4	N	123	GLY	2.8
5	O	136	SER	2.8
4	N	165	THR	2.8
5	O	212	LYS	2.8
4	K	208	SER	2.8
5	M	123	PHE	2.7
5	O	170	GLU	2.7
4	N	18	VAL	2.7
4	N	196	THR	2.7
5	O	156	ASP	2.7
5	O	189	ALA	2.7
5	O	213	SER	2.7
5	O	154	LYS	2.7
5	O	152	GLN	2.7
4	N	179	GLY	2.7
4	N	22	CYS	2.7
5	O	200	GLU	2.7
4	N	197	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	94	TYR	2.6
5	O	215	ASN	2.6
4	N	41	PRO	2.6
4	N	92	ALA	2.6
4	N	39	GLN	2.6
5	O	168	VAL	2.6
4	N	42	GLY	2.6
4	K	138	GLY	2.6
5	M	191	TYR	2.6
5	O	134	THR	2.6
4	N	122	LYS	2.6
5	O	121	PHE	2.6
4	N	209	ASN	2.6
4	J	194	LEU	2.5
4	K	150	TYR	2.5
4	K	199	TYR	2.5
4	N	169	HIS	2.5
2	H	47	GLU	2.5
5	O	184	LEU	2.5
2	H	0	MET	2.5
5	M	128	GLU	2.5
5	O	160	GLN	2.5
5	O	133	GLY	2.5
4	N	205	HIS	2.5
4	N	150	TYR	2.5
4	N	36	TRP	2.4
4	K	153	GLU	2.4
4	K	181	TYR	2.4
4	K	114	VAL	2.4
4	K	213	ASP	2.4
2	E	99	MET	2.4
5	O	195	LYS	2.4
1	G	172	LEU	2.4
2	E	94	LYS	2.4
4	K	81	MET	2.4
4	K	205	HIS	2.4
4	K	149	ASP	2.4
5	O	186	LEU	2.4
5	M	197	TYR	2.3
4	K	83	LEU	2.3
4	K	116	VAL	2.3
4	N	95	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	177	GLU	2.3
4	N	175	LEU	2.3
4	K	206	LYS	2.3
2	H	82	VAL	2.3
4	K	156	THR	2.2
4	K	219	LYS	2.2
4	N	164	LEU	2.2
5	O	206	LEU	2.2
2	H	98	ASP	2.2
4	K	86	LEU	2.2
4	N	108	TRP	2.2
4	N	177	SER	2.2
1	G	89	GLU	2.2
3	I	9	VAL	2.2
4	N	10	GLU	2.2
2	B	98	ASP	2.2
4	N	160	ASN	2.2
4	K	43	GLN	2.2
5	O	148	GLU	2.2
4	J	211	LYS	2.1
4	N	117	SER	2.1
4	N	178	SER	2.1
4	K	11	VAL	2.1
4	J	102	THR	2.1
2	E	87	LEU	2.1
5	M	214	PHE	2.1
4	J	56	VAL	2.1
4	K	18	VAL	2.1
1	D	272	LEU	2.1
1	D	227	ASP	2.1
5	O	43	GLN	2.1
5	O	191	TYR	2.1
4	N	192	SER	2.1
4	K	201	CYS	2.1
5	O	147	ARG	2.1
5	M	76	PHE	2.1
4	K	182	SER	2.0
4	N	202	ASN	2.0
5	M	126	SER	2.0
5	O	150	LYS	2.0
4	K	145	CYS	2.0
4	K	175	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	K	148	LYS	2.0
1	D	35	ARG	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.