



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:58 PM UTC

PDB ID : 9MQO / pdb_00009mqo
Title : Crystal structure of BCMA in complex with CA10v2 Fab
Authors : Qiu, Y.
Deposited on : 2025-01-04
Resolution : 3.18 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

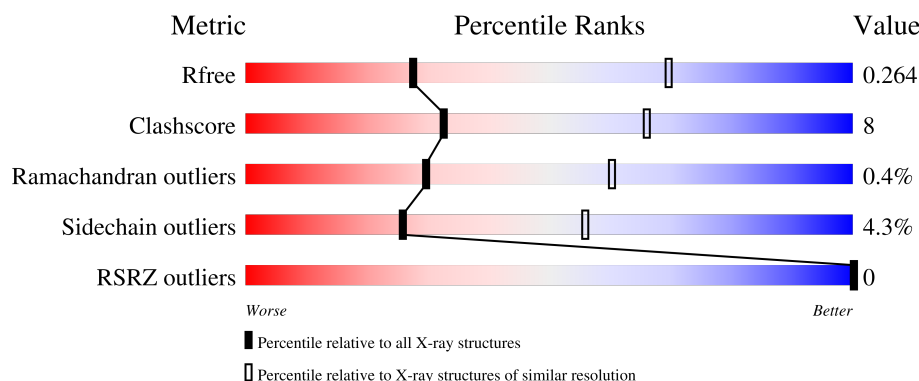
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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.



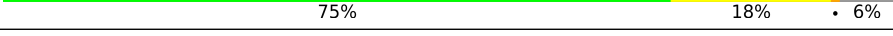
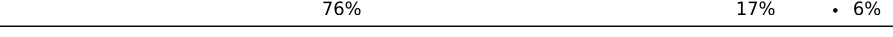
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	56	 55% 7% 36%
1	D	56	 55% 9% 36%
1	G	56	 55% 9% 36%
1	J	56	 57% 7% 36%
1	M	56	 54% 11% 36%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	56	
2	B	239	
2	E	239	
2	H	239	
2	K	239	
2	N	239	
2	Q	239	
3	C	216	
3	F	216	
3	I	216	
3	L	216	
3	O	216	
3	R	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20814 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 Tumor necrosis factor receptor superfamily member 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	36	Total	C	N	O	S	0	0	0
			280	170	50	54	6			
1	D	36	Total	C	N	O	S	0	0	0
			280	170	50	54	6			
1	G	36	Total	C	N	O	S	0	0	0
			280	170	50	54	6			
1	J	36	Total	C	N	O	S	0	0	0
			280	170	50	54	6			
1	M	36	Total	C	N	O	S	0	0	0
			280	170	50	54	6			
1	P	36	Total	C	N	O	S	0	0	0
			280	170	50	54	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q02223
A	0	PRO	-	expression tag	UNP Q02223
D	-1	GLY	-	expression tag	UNP Q02223
D	0	PRO	-	expression tag	UNP Q02223
G	-1	GLY	-	expression tag	UNP Q02223
G	0	PRO	-	expression tag	UNP Q02223
J	-1	GLY	-	expression tag	UNP Q02223
J	0	PRO	-	expression tag	UNP Q02223
M	-1	GLY	-	expression tag	UNP Q02223
M	0	PRO	-	expression tag	UNP Q02223
P	-1	GLY	-	expression tag	UNP Q02223
P	0	PRO	-	expression tag	UNP Q02223

- Molecule 2 is a protein called CA10v2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1650	1041	279	322	8			
2	E	217	Total	C	N	O	S	0	0	0
			1650	1041	279	322	8			
2	H	217	Total	C	N	O	S	0	0	0
			1650	1041	279	322	8			
2	K	217	Total	C	N	O	S	0	0	0
			1650	1041	279	322	8			
2	N	217	Total	C	N	O	S	0	0	0
			1650	1041	279	322	8			
2	Q	217	Total	C	N	O	S	0	0	0
			1650	1041	279	322	8			

- Molecule 3 is a protein called CA10v2 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	204	Total	C	N	O	S	0	0	0
			1539	967	258	309	5			
3	F	204	Total	C	N	O	S	0	0	0
			1539	967	258	309	5			
3	I	204	Total	C	N	O	S	0	0	0
			1539	967	258	309	5			
3	L	204	Total	C	N	O	S	0	0	0
			1539	967	258	309	5			
3	O	204	Total	C	N	O	S	0	0	0
			1539	967	258	309	5			
3	R	204	Total	C	N	O	S	0	0	0
			1539	967	258	309	5			

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: Tumor necrosis factor receptor superfamily member 17

Chain A: 



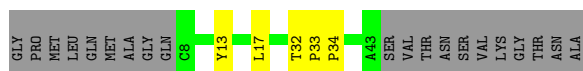
- Molecule 1: Tumor necrosis factor receptor superfamily member 17

Chain D: 



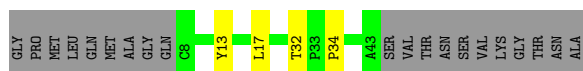
- Molecule 1: Tumor necrosis factor receptor superfamily member 17

Chain G: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 17

Chain J: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 17

Chain M: 



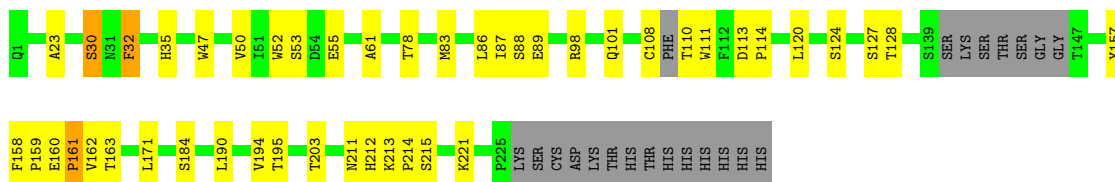
- Molecule 1: Tumor necrosis factor receptor superfamily member 17

Chain P: 



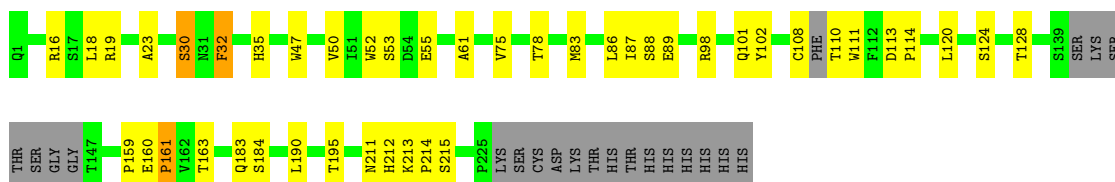
• Molecule 2: CA10v2 Fab heavy chain

Chain B: 72% 18% 9%



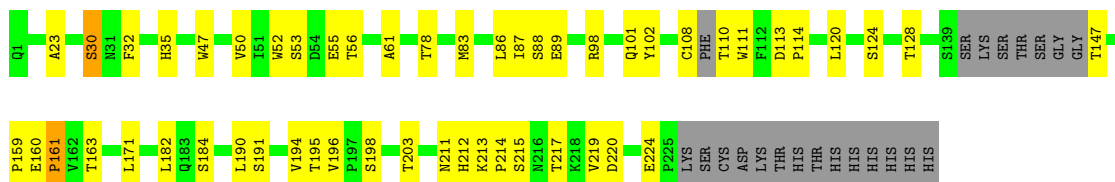
• Molecule 2: CA10v2 Fab heavy chain

Chain E: 72% 17% 9%



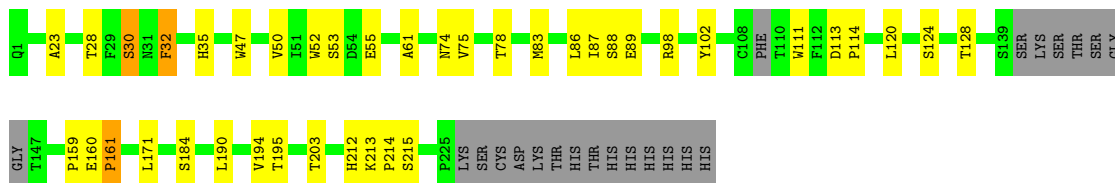
• Molecule 2: CA10v2 Fab heavy chain

Chain H: 69% 21% 9%



• Molecule 2: CA10v2 Fab heavy chain

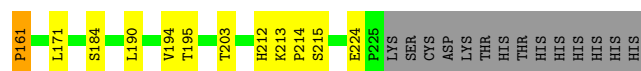
Chain K: 74% 15% 9%



• Molecule 2: CA10v2 Fab heavy chain

Chain N: 74% 15% 9%

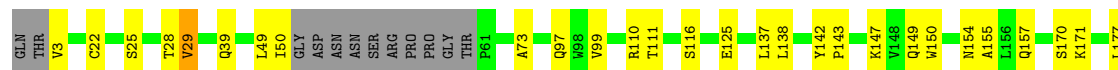
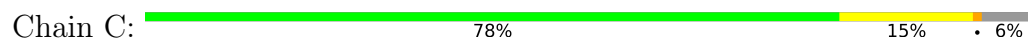




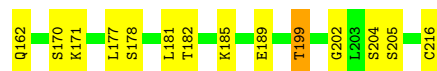
• Molecule 2: CA10v2 Fab heavy chain



• Molecule 3: CA10v2 Fab light chain



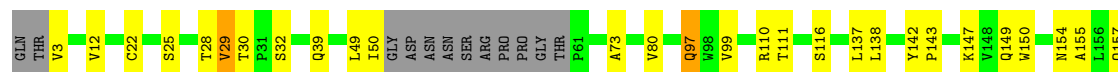
• Molecule 3: CA10v2 Fab light chain



• Molecule 3: CA10v2 Fab light chain

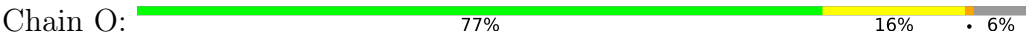


• Molecule 3: CA10v2 Fab light chain

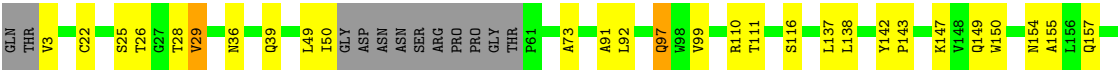




• Molecule 3: CA10v2 Fab light chain



• Molecule 3: CA10v2 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.16Å 94.78Å 108.13Å 81.39° 81.40° 62.67°	Depositor
Resolution (Å)	83.85 – 3.18 83.85 – 3.18	Depositor EDS
% Data completeness (in resolution range)	67.4 (83.85-3.18) 52.3 (83.85-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.232 , 0.272 0.241 , 0.264	Depositor DCC
R_{free} test set	1456 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.058 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20814	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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	1.01	0/286	1.47	0/389
1	D	1.01	0/286	1.49	0/389
1	G	1.03	0/286	1.49	0/389
1	J	1.02	0/286	1.49	0/389
1	M	1.03	0/286	1.48	0/389
1	P	1.03	0/286	1.48	0/389
2	B	1.00	0/1691	1.34	4/2307 (0.2%)
2	E	1.01	0/1691	1.34	4/2307 (0.2%)
2	H	1.00	0/1691	1.34	2/2307 (0.1%)
2	K	1.01	0/1691	1.33	4/2307 (0.2%)
2	N	1.00	0/1691	1.34	4/2307 (0.2%)
2	Q	1.01	0/1691	1.33	2/2307 (0.1%)
3	C	1.01	0/1573	1.30	0/2142
3	F	1.01	0/1573	1.31	0/2142
3	I	1.01	0/1573	1.31	0/2142
3	L	1.01	0/1573	1.30	0/2142
3	O	1.01	0/1573	1.31	0/2142
3	R	1.01	0/1573	1.31	0/2142
All	All	1.01	0/21300	1.33	20/29028 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	124	SER	CA-C-N	5.58	127.75	120.28
2	E	124	SER	C-N-CA	5.58	127.75	120.28
2	N	124	SER	CA-C-N	5.56	127.73	120.28
2	N	124	SER	C-N-CA	5.56	127.73	120.28
2	H	124	SER	CA-C-N	5.54	127.70	120.28
2	H	124	SER	C-N-CA	5.54	127.70	120.28
2	Q	124	SER	CA-C-N	5.40	127.51	120.28
2	Q	124	SER	C-N-CA	5.40	127.51	120.28
2	K	124	SER	CA-C-N	5.33	127.43	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	124	SER	C-N-CA	5.33	127.43	120.28
2	B	124	SER	CA-C-N	5.31	127.39	120.28
2	B	124	SER	C-N-CA	5.31	127.39	120.28
2	N	32	PHE	CA-C-N	5.24	125.07	120.10
2	N	32	PHE	C-N-CA	5.24	125.07	120.10
2	B	32	PHE	CA-C-N	5.13	124.98	120.10
2	B	32	PHE	C-N-CA	5.13	124.98	120.10
2	K	32	PHE	CA-C-N	5.04	124.89	120.10
2	K	32	PHE	C-N-CA	5.04	124.89	120.10
2	E	32	PHE	CA-C-N	5.04	124.89	120.10
2	E	32	PHE	C-N-CA	5.04	124.89	120.10

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	280	0	255	5	0
1	D	280	0	255	5	0
1	G	280	0	255	3	0
1	J	280	0	255	2	0
1	M	280	0	255	3	0
1	P	280	0	255	4	0
2	B	1650	0	1592	39	1
2	E	1650	0	1592	40	0
2	H	1650	0	1592	40	3
2	K	1650	0	1592	42	0
2	N	1650	0	1592	30	3
2	Q	1650	0	1592	47	0
3	C	1539	0	1498	16	0
3	F	1539	0	1498	22	2
3	I	1539	0	1498	18	0
3	L	1539	0	1498	17	0
3	O	1539	0	1498	23	0
3	R	1539	0	1498	21	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20814	0	20070	321	6

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 (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:K:74:ASN:O	2:Q:1:GLN:HB2	1.11	1.28
2:K:74:ASN:O	2:Q:1:GLN:CB	2.04	1.05
2:K:28:THR:HG22	2:Q:3:GLN:HE22	1.29	0.97
2:K:74:ASN:C	2:Q:1:GLN:HB2	1.98	0.88
3:L:3:VAL:N	3:L:25:SER:HG	1.75	0.84
3:C:3:VAL:N	3:C:25:SER:HG	1.75	0.84
2:E:214:PRO:O	2:H:224:GLU:OE2	1.97	0.82
3:I:3:VAL:N	3:I:25:SER:HG	1.78	0.82
3:O:3:VAL:N	3:O:25:SER:HG	1.79	0.80
3:F:3:VAL:N	3:F:25:SER:HG	1.79	0.80
3:R:3:VAL:N	3:R:25:SER:HG	1.81	0.79
2:K:28:THR:HG22	2:Q:3:GLN:NE2	1.99	0.78
2:K:30:SER:OG	2:Q:1:GLN:NE2	2.19	0.75
2:B:47:TRP:HZ2	2:B:50:VAL:HG23	1.54	0.72
2:H:47:TRP:HZ2	2:H:50:VAL:HG23	1.55	0.71
2:E:47:TRP:HZ2	2:E:50:VAL:HG23	1.55	0.71
2:N:47:TRP:HZ2	2:N:50:VAL:HG23	1.55	0.71
2:E:75:VAL:HG21	3:O:203:LEU:O	1.92	0.70
2:K:47:TRP:HZ2	2:K:50:VAL:HG23	1.56	0.70
2:K:120:LEU:HD21	2:K:160:GLU:HB2	1.74	0.70
2:Q:47:TRP:HZ2	2:Q:50:VAL:HG23	1.56	0.70
2:B:127:SER:HB2	3:F:204:SER:OG	1.92	0.69
2:E:120:LEU:HD21	2:E:160:GLU:HB2	1.75	0.68
2:Q:120:LEU:HD21	2:Q:160:GLU:HB2	1.75	0.68
2:N:120:LEU:HD21	2:N:160:GLU:HB2	1.75	0.67
2:Q:30:SER:O	2:Q:53:SER:HB2	1.95	0.67
2:E:30:SER:O	2:E:53:SER:HB2	1.95	0.66
2:H:120:LEU:HD21	2:H:160:GLU:HB2	1.76	0.66
2:K:30:SER:O	2:K:53:SER:HB2	1.95	0.66
2:B:30:SER:O	2:B:53:SER:HB2	1.95	0.66
2:N:30:SER:O	2:N:53:SER:HB2	1.95	0.66
2:H:30:SER:O	2:H:53:SER:HB2	1.96	0.66
2:E:16:ARG:HB3	2:H:220:ASP:OD2	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:74:ASN:C	2:Q:1:GLN:CB	2.64	0.63
2:B:120:LEU:HD21	2:B:160:GLU:HB2	1.80	0.63
2:Q:128:THR:HG23	2:Q:159:PRO:HG2	1.81	0.62
2:K:128:THR:HG23	2:K:159:PRO:HG2	1.82	0.62
2:B:128:THR:HG23	2:B:159:PRO:HG2	1.82	0.61
3:I:155:ALA:O	3:I:157:GLN:NE2	2.34	0.60
2:H:128:THR:HG23	2:H:159:PRO:HG2	1.82	0.60
2:K:120:LEU:CD2	2:K:160:GLU:HB2	2.31	0.60
2:N:111:TRP:HB3	3:O:50:ILE:HD11	1.84	0.60
2:E:120:LEU:CD2	2:E:160:GLU:HB2	2.31	0.60
3:R:155:ALA:O	3:R:157:GLN:NE2	2.35	0.60
2:H:182:LEU:HD21	3:O:110:ARG:C	2.27	0.60
2:E:128:THR:HG23	2:E:159:PRO:HG2	1.84	0.60
2:H:98:ARG:HB3	2:H:114:PRO:HG3	1.82	0.60
2:N:120:LEU:CD2	2:N:160:GLU:HB2	2.32	0.59
3:F:155:ALA:O	3:F:157:GLN:NE2	2.34	0.59
2:K:98:ARG:HB3	2:K:114:PRO:HG3	1.83	0.59
2:N:98:ARG:HB3	2:N:114:PRO:HG3	1.84	0.59
3:L:155:ALA:O	3:L:157:GLN:NE2	2.35	0.59
2:N:128:THR:HG23	2:N:159:PRO:HG2	1.83	0.59
2:B:98:ARG:HB3	2:B:114:PRO:HG3	1.84	0.59
2:H:98:ARG:HB3	2:H:114:PRO:CG	2.32	0.59
3:C:155:ALA:O	3:C:157:GLN:NE2	2.35	0.59
2:E:98:ARG:HB3	2:E:114:PRO:HG3	1.85	0.59
2:Q:120:LEU:CD2	2:Q:160:GLU:HB2	2.33	0.59
3:O:155:ALA:O	3:O:157:GLN:NE2	2.35	0.58
2:K:98:ARG:HB3	2:K:114:PRO:CG	2.33	0.58
2:Q:98:ARG:HB3	2:Q:114:PRO:HG3	1.84	0.58
2:B:127:SER:N	3:F:202:GLY:O	2.37	0.58
2:H:120:LEU:CD2	2:H:160:GLU:HB2	2.34	0.58
2:B:120:LEU:CD2	2:B:160:GLU:HB2	2.33	0.58
2:B:98:ARG:HB3	2:B:114:PRO:CG	2.34	0.58
2:N:98:ARG:HB3	2:N:114:PRO:CG	2.34	0.58
2:Q:98:ARG:HB3	2:Q:114:PRO:CG	2.34	0.58
2:B:127:SER:OG	3:F:204:SER:N	2.38	0.57
2:Q:111:TRP:HB3	3:R:50:ILE:HD11	1.87	0.56
2:E:98:ARG:HB3	2:E:114:PRO:CG	2.35	0.56
2:Q:47:TRP:CZ3	3:R:97:GLN:HB2	2.42	0.55
1:G:17:LEU:HB2	2:H:102:TYR:HB2	1.88	0.55
1:A:32:THR:O	2:B:108:CYS:HB2	2.06	0.54
1:A:33:PRO:C	2:B:108:CYS:HB3	2.33	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:185:LYS:O	3:O:189:GLU:HG2	2.08	0.54
3:L:185:LYS:O	3:L:189:GLU:HG2	2.08	0.54
3:I:185:LYS:O	3:I:189:GLU:HG2	2.08	0.53
3:L:22:CYS:HB3	3:L:73:ALA:HB3	1.90	0.53
2:K:75:VAL:O	2:Q:1:GLN:N	2.42	0.53
3:C:185:LYS:O	3:C:189:GLU:HG2	2.09	0.53
3:F:22:CYS:HB3	3:F:73:ALA:HB3	1.91	0.53
3:F:185:LYS:O	3:F:189:GLU:HG2	2.08	0.53
2:H:190:LEU:HD12	2:H:190:LEU:C	2.33	0.53
3:C:22:CYS:HB3	3:C:73:ALA:HB3	1.90	0.53
2:N:190:LEU:C	2:N:190:LEU:HD12	2.33	0.53
2:Q:101:GLN:HG2	2:Q:110:THR:HG22	1.91	0.52
3:R:185:LYS:O	3:R:189:GLU:HG2	2.08	0.52
2:B:190:LEU:C	2:B:190:LEU:HD12	2.35	0.52
3:I:22:CYS:HB3	3:I:73:ALA:HB3	1.91	0.52
2:Q:190:LEU:C	2:Q:190:LEU:HD12	2.34	0.52
2:K:47:TRP:CZ3	3:L:97:GLN:HB2	2.45	0.52
2:E:190:LEU:HD12	2:E:190:LEU:C	2.34	0.52
2:E:47:TRP:CZ2	2:E:50:VAL:HG23	2.42	0.52
3:R:22:CYS:HB3	3:R:73:ALA:HB3	1.91	0.52
1:D:17:LEU:HB2	2:E:102:TYR:HB2	1.92	0.52
3:O:22:CYS:HB3	3:O:73:ALA:HB3	1.91	0.51
3:R:110:ARG:NH2	3:R:111:THR:HG23	2.25	0.51
3:F:110:ARG:NH2	3:F:111:THR:HG23	2.25	0.51
3:C:110:ARG:NH2	3:C:111:THR:HG23	2.25	0.51
2:K:190:LEU:C	2:K:190:LEU:HD12	2.34	0.51
1:P:33:PRO:C	2:Q:108:CYS:HB3	2.35	0.51
3:L:110:ARG:NH2	3:L:111:THR:HG23	2.26	0.51
2:E:35:HIS:ND1	2:E:50:VAL:HG22	2.26	0.51
2:H:47:TRP:CZ3	3:I:97:GLN:HB2	2.46	0.50
2:H:101:GLN:HG2	2:H:110:THR:HG22	1.93	0.50
3:I:110:ARG:NH2	3:I:111:THR:HG23	2.26	0.50
2:B:47:TRP:CZ2	2:B:50:VAL:HG23	2.42	0.50
2:B:35:HIS:ND1	2:B:50:VAL:HG22	2.27	0.50
2:N:23:ALA:HA	2:N:78:THR:HG22	1.94	0.50
1:D:33:PRO:C	2:E:108:CYS:HB3	2.37	0.49
3:O:138:LEU:HD12	3:O:138:LEU:N	2.27	0.49
2:E:32:PHE:CD1	2:E:98:ARG:HD2	2.47	0.49
2:N:101:GLN:HG2	2:N:110:THR:HG22	1.92	0.49
2:K:32:PHE:CD1	2:K:98:ARG:HD2	2.47	0.49
1:M:17:LEU:HB2	2:N:102:TYR:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:83:MET:HB3	2:K:86:LEU:HD21	1.95	0.49
2:Q:52:TRP:HB2	2:Q:55:GLU:HB2	1.95	0.49
2:E:19:ARG:NH1	2:H:217:THR:OG1	2.46	0.49
2:E:23:ALA:HA	2:E:78:THR:HG22	1.94	0.49
2:K:35:HIS:ND1	2:K:50:VAL:HG22	2.28	0.49
2:B:32:PHE:CD1	2:B:98:ARG:HD2	2.48	0.49
2:K:23:ALA:HA	2:K:78:THR:HG22	1.95	0.49
3:I:138:LEU:N	3:I:138:LEU:HD12	2.28	0.49
3:C:138:LEU:HD12	3:C:138:LEU:N	2.28	0.48
2:H:32:PHE:CD1	2:H:98:ARG:HD2	2.47	0.48
1:J:17:LEU:HB2	2:K:102:TYR:HB2	1.94	0.48
3:O:110:ARG:NH2	3:O:111:THR:HG23	2.27	0.48
2:N:35:HIS:ND1	2:N:50:VAL:HG22	2.28	0.48
3:O:147:LYS:HB3	3:O:199:THR:HB	1.95	0.48
3:R:138:LEU:HD12	3:R:138:LEU:N	2.28	0.48
3:F:138:LEU:HD12	3:F:138:LEU:N	2.28	0.48
2:H:35:HIS:ND1	2:H:50:VAL:HG22	2.28	0.48
3:L:138:LEU:N	3:L:138:LEU:HD12	2.28	0.48
2:B:221:LYS:NZ	3:C:125:GLU:OE2	2.43	0.48
3:C:147:LYS:HB3	3:C:199:THR:HB	1.96	0.48
2:Q:87:ILE:HB	2:Q:89:GLU:HG3	1.96	0.48
2:H:23:ALA:HA	2:H:78:THR:HG22	1.95	0.48
2:H:47:TRP:CZ2	2:H:50:VAL:HG23	2.43	0.48
2:Q:23:ALA:HA	2:Q:78:THR:HG22	1.95	0.48
3:I:147:LYS:HB3	3:I:199:THR:HB	1.96	0.48
2:N:87:ILE:HB	2:N:89:GLU:HG3	1.96	0.48
2:N:213:LYS:HB2	2:N:214:PRO:HD3	1.95	0.48
2:Q:32:PHE:CD1	2:Q:98:ARG:HD2	2.48	0.48
2:Q:160:GLU:N	2:Q:161:PRO:CD	2.77	0.48
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.96	0.47
2:B:87:ILE:HB	2:B:89:GLU:HG3	1.95	0.47
3:C:142:TYR:CG	3:C:143:PRO:HA	2.49	0.47
2:E:101:GLN:HG2	2:E:110:THR:HG22	1.95	0.47
2:H:160:GLU:N	2:H:161:PRO:CD	2.77	0.47
2:N:32:PHE:CD1	2:N:98:ARG:HD2	2.49	0.47
1:P:32:THR:O	2:Q:108:CYS:HB2	2.15	0.47
2:K:87:ILE:HB	2:K:89:GLU:HG3	1.97	0.47
2:Q:35:HIS:ND1	2:Q:50:VAL:HG22	2.28	0.47
2:N:47:TRP:CZ2	2:N:50:VAL:HG23	2.43	0.47
3:O:142:TYR:CG	3:O:143:PRO:HA	2.49	0.47
2:E:213:LYS:HB2	2:E:214:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:ARG:CB	2:H:114:PRO:HG3	2.45	0.47
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.95	0.47
2:B:160:GLU:N	2:B:161:PRO:CD	2.78	0.47
2:E:87:ILE:HB	2:E:89:GLU:HG3	1.96	0.47
2:H:213:LYS:HB2	2:H:214:PRO:HD3	1.96	0.47
2:K:98:ARG:CB	2:K:114:PRO:HG3	2.45	0.47
3:L:147:LYS:HB3	3:L:199:THR:HB	1.97	0.47
2:N:52:TRP:HB2	2:N:55:GLU:HB2	1.96	0.47
2:H:111:TRP:HB3	3:I:50:ILE:HD11	1.97	0.47
2:N:160:GLU:N	2:N:161:PRO:CD	2.77	0.47
2:B:52:TRP:HB2	2:B:55:GLU:HB2	1.96	0.47
3:I:142:TYR:CG	3:I:143:PRO:HA	2.50	0.47
3:L:142:TYR:CG	3:L:143:PRO:HA	2.50	0.47
3:O:137:LEU:C	3:O:138:LEU:HD12	2.40	0.47
2:Q:213:LYS:HB2	2:Q:214:PRO:HD3	1.96	0.47
3:R:142:TYR:CG	3:R:143:PRO:HA	2.50	0.46
2:B:23:ALA:HA	2:B:78:THR:HG22	1.96	0.46
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.96	0.46
2:K:111:TRP:HB3	3:L:50:ILE:HD11	1.97	0.46
2:K:160:GLU:N	2:K:161:PRO:CD	2.78	0.46
2:E:160:GLU:N	2:E:161:PRO:CD	2.79	0.46
2:N:83:MET:HB3	2:N:86:LEU:HD21	1.96	0.46
3:C:137:LEU:C	3:C:138:LEU:HD12	2.41	0.46
2:Q:83:MET:HB3	2:Q:86:LEU:HD21	1.96	0.46
2:H:87:ILE:HB	2:H:89:GLU:HG3	1.97	0.46
2:E:47:TRP:CZ3	3:F:97:GLN:HB2	2.51	0.46
2:N:98:ARG:CB	2:N:114:PRO:HG3	2.45	0.46
2:Q:47:TRP:CZ2	2:Q:50:VAL:HG23	2.43	0.46
2:B:47:TRP:CE3	2:B:61:ALA:HB2	2.50	0.46
2:H:52:TRP:HB2	2:H:55:GLU:HB2	1.98	0.46
2:E:52:TRP:HB2	2:E:55:GLU:HB2	1.97	0.46
3:L:137:LEU:C	3:L:138:LEU:HD12	2.41	0.46
3:R:147:LYS:HB3	3:R:199:THR:HB	1.98	0.46
2:B:158:PHE:CD1	3:F:112:VAL:CG1	2.99	0.45
2:N:171:LEU:HD21	2:N:194:VAL:HG21	1.98	0.45
2:N:47:TRP:CE3	2:N:61:ALA:HB2	2.51	0.45
2:Q:47:TRP:CE3	2:Q:61:ALA:HB2	2.51	0.45
3:R:28:THR:HG22	3:R:29:VAL:O	2.17	0.45
1:D:34:PRO:N	2:E:108:CYS:HB3	2.31	0.45
2:H:47:TRP:CE3	2:H:61:ALA:HB2	2.51	0.45
3:I:137:LEU:C	3:I:138:LEU:HD12	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:47:TRP:CE3	2:K:61:ALA:HB2	2.52	0.45
2:K:52:TRP:HB2	2:K:55:GLU:HB2	1.97	0.45
2:Q:183:GLN:HA	3:R:162:GLN:HE22	1.81	0.45
1:A:34:PRO:HD3	2:B:108:CYS:SG	2.57	0.45
2:B:213:LYS:HB2	2:B:214:PRO:HD3	1.99	0.45
3:I:150:TRP:CE2	3:I:181:LEU:HB2	2.52	0.45
2:N:111:TRP:HB3	3:O:50:ILE:CD1	2.46	0.45
3:O:150:TRP:CE2	3:O:181:LEU:HB2	2.52	0.45
2:B:111:TRP:HB3	3:C:50:ILE:HD11	1.97	0.45
2:E:47:TRP:CE3	2:E:61:ALA:HB2	2.51	0.45
3:L:28:THR:HG22	3:L:29:VAL:O	2.17	0.45
3:F:142:TYR:CG	3:F:143:PRO:HA	2.50	0.45
2:E:98:ARG:CB	2:E:114:PRO:HG3	2.45	0.45
2:E:183:GLN:HA	3:F:162:GLN:HE22	1.82	0.45
2:K:213:LYS:HB2	2:K:214:PRO:HD3	1.98	0.45
3:F:137:LEU:C	3:F:138:LEU:HD12	2.42	0.45
3:F:150:TRP:CE2	3:F:181:LEU:HB2	2.52	0.45
3:L:150:TRP:CE2	3:L:181:LEU:HB2	2.52	0.45
3:C:150:TRP:CE2	3:C:181:LEU:HB2	2.52	0.44
3:L:39:GLN:HB2	3:L:49:LEU:HD11	1.99	0.44
3:C:39:GLN:HB2	3:C:49:LEU:HD11	1.99	0.44
1:D:34:PRO:HD3	2:E:108:CYS:SG	2.57	0.44
3:R:39:GLN:HB2	3:R:49:LEU:HD11	1.99	0.44
3:R:137:LEU:C	3:R:138:LEU:HD12	2.42	0.44
3:R:150:TRP:CE2	3:R:181:LEU:HB2	2.52	0.44
2:B:163:THR:HB	2:B:211:ASN:HB3	1.99	0.44
3:I:28:THR:HG22	3:I:29:VAL:O	2.18	0.44
3:O:28:THR:HG22	3:O:29:VAL:O	2.18	0.44
3:O:39:GLN:HB2	3:O:49:LEU:HD11	2.00	0.44
2:B:98:ARG:CB	2:B:114:PRO:HG3	2.46	0.44
3:F:147:LYS:HB3	3:F:199:THR:HB	1.99	0.44
2:Q:98:ARG:CB	2:Q:114:PRO:HG3	2.46	0.44
3:F:28:THR:HG22	3:F:29:VAL:O	2.17	0.44
3:I:39:GLN:HB2	3:I:49:LEU:HD11	1.99	0.44
1:A:10:GLN:NE2	1:P:25:GLN:OE1	2.48	0.43
3:R:36:ASN:HB2	3:R:50:ILE:HG12	1.99	0.43
2:E:110:THR:O	3:F:36:ASN:HB3	2.19	0.43
2:E:111:TRP:HB3	3:F:50:ILE:HD11	2.01	0.43
3:F:39:GLN:HB2	3:F:49:LEU:HD11	2.00	0.43
2:K:30:SER:HG	2:Q:1:GLN:HE22	1.65	0.43
3:O:36:ASN:HB2	3:O:50:ILE:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2:VAL:HA	2:Q:26:GLY:HA3	2.01	0.43
3:C:28:THR:HG22	3:C:29:VAL:O	2.18	0.43
2:K:47:TRP:CZ2	2:K:50:VAL:HG23	2.43	0.43
2:K:159:PRO:HD2	2:K:212:HIS:HE1	1.84	0.43
2:N:159:PRO:HB2	2:N:214:PRO:HG2	2.01	0.43
2:E:18:LEU:HD12	2:H:219:VAL:HG13	2.00	0.43
2:K:32:PHE:HB3	2:K:98:ARG:HG3	2.01	0.43
2:B:101:GLN:HG2	2:B:110:THR:HG22	2.00	0.42
3:F:177:LEU:HG	3:F:178:SER:N	2.33	0.42
2:B:113:ASP:N	2:B:114:PRO:HD2	2.35	0.42
3:C:177:LEU:HG	3:C:178:SER:N	2.35	0.42
2:E:163:THR:HB	2:E:211:ASN:HB3	2.01	0.42
2:N:47:TRP:CZ3	3:O:97:GLN:HB2	2.54	0.42
3:O:177:LEU:HG	3:O:178:SER:N	2.33	0.42
2:H:182:LEU:HD21	3:O:111:THR:N	2.34	0.42
2:K:160:GLU:N	2:K:161:PRO:HD3	2.34	0.42
2:Q:113:ASP:N	2:Q:114:PRO:HD2	2.35	0.42
2:Q:159:PRO:HB2	2:Q:214:PRO:HG2	2.01	0.42
2:E:212:HIS:ND1	2:E:215:SER:HB3	2.35	0.42
2:H:113:ASP:N	2:H:114:PRO:HD2	2.35	0.42
2:K:159:PRO:HB2	2:K:214:PRO:HG2	2.01	0.42
2:K:75:VAL:HA	2:Q:1:GLN:H3	1.84	0.42
2:N:212:HIS:ND1	2:N:215:SER:HB3	2.35	0.42
2:Q:212:HIS:ND1	2:Q:215:SER:HB3	2.35	0.42
2:H:171:LEU:HD21	2:H:194:VAL:HG21	2.02	0.42
3:I:177:LEU:HG	3:I:178:SER:N	2.35	0.42
3:R:177:LEU:HG	3:R:178:SER:N	2.35	0.42
2:E:113:ASP:N	2:E:114:PRO:HD2	2.35	0.41
2:H:212:HIS:ND1	2:H:215:SER:HB3	2.35	0.41
2:K:159:PRO:HD2	2:K:212:HIS:CE1	2.54	0.41
2:H:163:THR:HB	2:H:211:ASN:HB3	2.02	0.41
3:I:36:ASN:HB2	3:I:50:ILE:HG12	2.03	0.41
3:R:178:SER:O	3:R:178:SER:OG	2.37	0.41
1:G:33:PRO:C	2:H:108:CYS:HB3	2.45	0.41
2:Q:159:PRO:HD2	2:Q:212:HIS:CE1	2.55	0.41
2:B:160:GLU:N	2:B:161:PRO:HD3	2.35	0.41
2:E:159:PRO:HD2	2:E:212:HIS:HE1	1.85	0.41
2:H:32:PHE:HB3	2:H:98:ARG:HG3	2.02	0.41
2:K:171:LEU:HD21	2:K:194:VAL:HG21	2.01	0.41
2:Q:159:PRO:HD2	2:Q:212:HIS:HE1	1.85	0.41
1:A:13:TYR:CE1	1:A:34:PRO:HG2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:TYR:CE1	1:J:34:PRO:HG2	2.56	0.41
2:K:212:HIS:ND1	2:K:215:SER:HB3	2.35	0.41
1:M:13:TYR:CE1	1:M:34:PRO:HG2	2.56	0.41
2:N:111:TRP:HB3	3:O:50:ILE:CG1	2.49	0.41
2:Q:171:LEU:HD21	2:Q:194:VAL:HG21	2.03	0.41
2:B:159:PRO:HB2	2:B:214:PRO:HG2	2.02	0.41
2:Q:181:VAL:CG1	3:R:164:SER:HB2	2.50	0.41
3:R:91:ALA:O	3:R:92:LEU:HD12	2.21	0.41
2:H:160:GLU:N	2:H:161:PRO:HD3	2.36	0.41
3:I:91:ALA:O	3:I:92:LEU:HD12	2.21	0.41
3:R:3:VAL:O	3:R:25:SER:HB3	2.21	0.41
2:B:159:PRO:HD2	2:B:212:HIS:CE1	2.56	0.41
2:B:212:HIS:ND1	2:B:215:SER:HB3	2.36	0.41
1:D:13:TYR:CE1	1:D:34:PRO:HG2	2.55	0.41
2:E:159:PRO:HD2	2:E:212:HIS:CE1	2.56	0.41
2:E:160:GLU:N	2:E:161:PRO:HD3	2.36	0.41
2:H:32:PHE:CG	2:H:98:ARG:HD2	2.56	0.41
2:H:159:PRO:HD2	2:H:212:HIS:HE1	1.86	0.41
2:K:113:ASP:N	2:K:114:PRO:HD2	2.36	0.41
2:N:159:PRO:HD2	2:N:212:HIS:CE1	2.56	0.41
3:O:3:VAL:O	3:O:25:SER:HB3	2.21	0.41
2:Q:163:THR:HB	2:Q:211:ASN:HB3	2.02	0.41
2:H:159:PRO:HD2	2:H:212:HIS:CE1	2.56	0.41
3:I:3:VAL:O	3:I:25:SER:HB3	2.21	0.41
2:K:74:ASN:C	2:Q:1:GLN:HB3	2.45	0.41
1:M:33:PRO:C	2:N:108:CYS:HB3	2.46	0.41
2:B:32:PHE:HB3	2:B:98:ARG:HG3	2.04	0.40
2:B:171:LEU:HD21	2:B:194:VAL:HG21	2.01	0.40
3:L:177:LEU:HG	3:L:178:SER:N	2.35	0.40
1:P:34:PRO:N	2:Q:108:CYS:HB3	2.35	0.40
2:B:157:TYR:CE2	2:B:162:VAL:HG23	2.56	0.40
3:F:91:ALA:O	3:F:92:LEU:HD12	2.21	0.40
1:G:13:TYR:CE1	1:G:34:PRO:HG2	2.55	0.40
2:Q:98:ARG:O	2:Q:112:PHE:HA	2.21	0.40
2:E:159:PRO:HB2	2:E:214:PRO:HG2	2.03	0.40
2:H:147:THR:N	2:H:198:SER:HG	2.20	0.40
2:B:159:PRO:HD2	2:B:212:HIS:HE1	1.85	0.40
3:C:178:SER:O	3:C:178:SER:OG	2.36	0.40
2:K:32:PHE:CG	2:K:98:ARG:HD2	2.57	0.40
3:L:12:VAL:HG13	3:L:80:VAL:HG21	2.04	0.40
3:L:30:THR:OG1	3:L:32:SER:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:91:ALA:O	3:O:92:LEU:HD12	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:PRO:O	2:N:224:GLU:OE2[1_554]	1.92	0.28
2:H:56:THR:OG1	3:R:26:THR:CG2[1_546]	1.95	0.25
2:H:203:THR:O	3:R:204:SER:C[1_545]	1.96	0.24
3:F:204:SER:C	2:N:203:THR:O[1_554]	2.05	0.15
2:H:203:THR:O	3:R:204:SER:O[1_545]	2.06	0.14
3:F:205:SER:N	2:N:203:THR:O[1_554]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	34/56 (61%)	31 (91%)	3 (9%)	0	100	100
1	D	34/56 (61%)	31 (91%)	3 (9%)	0	100	100
1	G	34/56 (61%)	31 (91%)	3 (9%)	0	100	100
1	J	34/56 (61%)	31 (91%)	3 (9%)	0	100	100
1	M	34/56 (61%)	31 (91%)	3 (9%)	0	100	100
1	P	34/56 (61%)	30 (88%)	4 (12%)	0	100	100
2	B	211/239 (88%)	199 (94%)	11 (5%)	1 (0%)	24	57
2	E	211/239 (88%)	198 (94%)	12 (6%)	1 (0%)	24	57
2	H	211/239 (88%)	198 (94%)	12 (6%)	1 (0%)	24	57
2	K	211/239 (88%)	199 (94%)	11 (5%)	1 (0%)	24	57
2	N	211/239 (88%)	199 (94%)	11 (5%)	1 (0%)	24	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	211/239 (88%)	198 (94%)	12 (6%)	1 (0%)	24	57
3	C	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
3	F	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
3	I	200/216 (93%)	190 (95%)	9 (4%)	1 (0%)	24	57
3	L	200/216 (93%)	190 (95%)	9 (4%)	1 (0%)	24	57
3	O	200/216 (93%)	190 (95%)	9 (4%)	1 (0%)	24	57
3	R	200/216 (93%)	190 (95%)	9 (4%)	1 (0%)	24	57
All	All	2670/3066 (87%)	2518 (94%)	142 (5%)	10 (0%)	30	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	161	PRO
3	I	204	SER
3	L	204	SER
3	O	204	SER
3	R	204	SER
2	B	161	PRO
2	K	161	PRO
2	H	161	PRO
2	N	161	PRO
2	Q	161	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	34/49 (69%)	33 (97%)	1 (3%)	37	64
1	D	34/49 (69%)	33 (97%)	1 (3%)	37	64
1	G	34/49 (69%)	33 (97%)	1 (3%)	37	64
1	J	34/49 (69%)	33 (97%)	1 (3%)	37	64
1	M	34/49 (69%)	32 (94%)	2 (6%)	18	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	34/49 (69%)	33 (97%)	1 (3%)	37	64
2	B	187/207 (90%)	182 (97%)	5 (3%)	39	65
2	E	187/207 (90%)	183 (98%)	4 (2%)	47	69
2	H	187/207 (90%)	181 (97%)	6 (3%)	34	62
2	K	187/207 (90%)	182 (97%)	5 (3%)	39	65
2	N	187/207 (90%)	183 (98%)	4 (2%)	47	69
2	Q	187/207 (90%)	182 (97%)	5 (3%)	39	65
3	C	172/182 (94%)	161 (94%)	11 (6%)	16	44
3	F	172/182 (94%)	161 (94%)	11 (6%)	16	44
3	I	172/182 (94%)	161 (94%)	11 (6%)	16	44
3	L	172/182 (94%)	161 (94%)	11 (6%)	16	44
3	O	172/182 (94%)	162 (94%)	10 (6%)	18	47
3	R	172/182 (94%)	161 (94%)	11 (6%)	16	44
All	All	2358/2628 (90%)	2257 (96%)	101 (4%)	26	56

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
2	B	30	SER
2	B	88	SER
2	B	184	SER
2	B	195	THR
2	B	203	THR
3	C	29	VAL
3	C	97	GLN
3	C	99	VAL
3	C	116	SER
3	C	149	GLN
3	C	154	ASN
3	C	170	SER
3	C	171	LYS
3	C	182	THR
3	C	199	THR
3	C	216	CYS
1	D	32	THR
2	E	30	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	88	SER
2	E	184	SER
2	E	195	THR
3	F	29	VAL
3	F	97	GLN
3	F	99	VAL
3	F	116	SER
3	F	149	GLN
3	F	154	ASN
3	F	170	SER
3	F	171	LYS
3	F	182	THR
3	F	199	THR
3	F	216	CYS
1	G	32	THR
2	H	30	SER
2	H	88	SER
2	H	184	SER
2	H	191	SER
2	H	195	THR
2	H	196	VAL
3	I	29	VAL
3	I	97	GLN
3	I	99	VAL
3	I	116	SER
3	I	149	GLN
3	I	154	ASN
3	I	170	SER
3	I	171	LYS
3	I	182	THR
3	I	199	THR
3	I	216	CYS
1	J	32	THR
2	K	30	SER
2	K	88	SER
2	K	184	SER
2	K	195	THR
2	K	203	THR
3	L	29	VAL
3	L	97	GLN
3	L	99	VAL
3	L	116	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	149	GLN
3	L	154	ASN
3	L	170	SER
3	L	171	LYS
3	L	182	THR
3	L	199	THR
3	L	216	CYS
1	M	10	GLN
1	M	32	THR
2	N	30	SER
2	N	88	SER
2	N	184	SER
2	N	195	THR
3	O	29	VAL
3	O	97	GLN
3	O	99	VAL
3	O	116	SER
3	O	149	GLN
3	O	154	ASN
3	O	170	SER
3	O	182	THR
3	O	199	THR
3	O	216	CYS
1	P	32	THR
2	Q	30	SER
2	Q	88	SER
2	Q	184	SER
2	Q	195	THR
2	Q	203	THR
3	R	29	VAL
3	R	97	GLN
3	R	99	VAL
3	R	116	SER
3	R	149	GLN
3	R	154	ASN
3	R	170	SER
3	R	171	LYS
3	R	182	THR
3	R	199	THR
3	R	216	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
2	B	1	GLN
2	B	13	GLN
2	B	31	ASN
2	B	39	GLN
2	B	183	GLN
3	C	40	GLN
3	C	44	GLN
3	C	81	GLN
1	D	38	GLN
2	E	1	GLN
2	E	13	GLN
2	E	31	ASN
2	E	39	GLN
3	F	40	GLN
3	F	44	GLN
3	F	81	GLN
3	F	162	GLN
1	G	38	GLN
2	H	1	GLN
2	H	31	ASN
2	H	183	GLN
3	I	40	GLN
3	I	44	GLN
3	I	81	GLN
3	I	162	GLN
1	J	38	GLN
2	K	1	GLN
2	K	31	ASN
2	K	39	GLN
2	K	183	GLN
3	L	40	GLN
3	L	44	GLN
3	L	81	GLN
1	M	38	GLN
2	N	1	GLN
2	N	31	ASN
2	N	39	GLN
2	N	183	GLN
3	O	40	GLN
3	O	44	GLN
3	O	81	GLN
3	O	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	38	GLN
2	Q	1	GLN
2	Q	13	GLN
2	Q	31	ASN
2	Q	176	HIS
2	Q	183	GLN
3	R	40	GLN
3	R	44	GLN
3	R	81	GLN
3	R	162	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	36/56 (64%)	-1.74	0 100 100	71, 93, 113, 120	0
1	D	36/56 (64%)	-1.72	0 100 100	78, 106, 130, 139	0
1	G	36/56 (64%)	-1.70	0 100 100	83, 109, 133, 178	0
1	J	36/56 (64%)	-1.63	0 100 100	83, 108, 147, 155	0
1	M	36/56 (64%)	-1.49	0 100 100	102, 156, 204, 229	0
1	P	36/56 (64%)	-1.63	0 100 100	80, 107, 154, 172	0
2	B	217/239 (90%)	-1.83	0 100 100	26, 45, 77, 121	0
2	E	217/239 (90%)	-1.78	0 100 100	26, 53, 90, 131	0
2	H	217/239 (90%)	-1.75	0 100 100	35, 59, 106, 148	0
2	K	217/239 (90%)	-1.75	0 100 100	42, 72, 107, 173	0
2	N	217/239 (90%)	-1.76	0 100 100	31, 73, 137, 181	0
2	Q	217/239 (90%)	-1.71	0 100 100	45, 79, 117, 177	0
3	C	204/216 (94%)	-1.79	0 100 100	32, 52, 81, 106	0
3	F	204/216 (94%)	-1.82	0 100 100	27, 54, 77, 134	0
3	I	204/216 (94%)	-1.79	0 100 100	40, 61, 88, 118	0
3	L	204/216 (94%)	-1.77	0 100 100	33, 65, 94, 157	0
3	O	204/216 (94%)	-1.75	0 100 100	31, 62, 120, 152	0
3	R	204/216 (94%)	-1.77	0 100 100	38, 68, 103, 150	0
All	All	2742/3066 (89%)	-1.76	0 100 100	26, 64, 119, 229	0

There are no RSRZ outliers to report.

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 [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.