



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:35 PM GMT

PDB ID : 4FAO
Title : Specificity and Structure of a high affinity Activin-like 1 (ALK1) signaling complex
Authors : Townson, S.A.; Martinez-Hackert, E.; Greppi, C.; Lowden, P.; Sako, D.; Liu, J.; Ucran, J.A.; Liharska, K.; Underwood, K.W.; Seehra, J.; Kumar, R.; Grinberg, A.V.
Deposited on : 2012-05-22
Resolution : 3.36 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

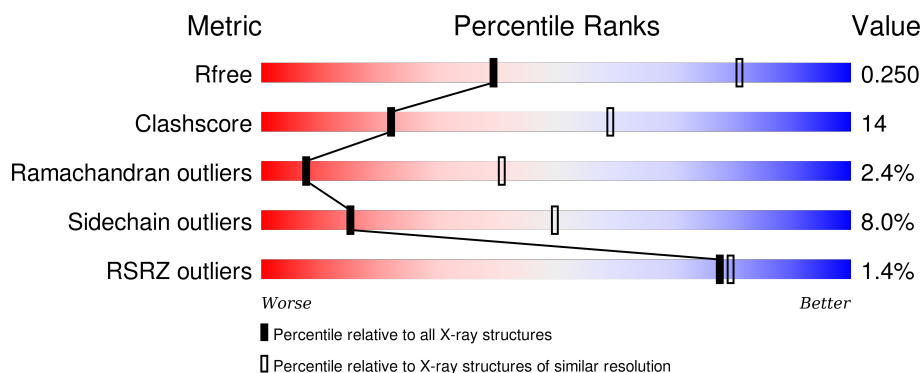
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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.














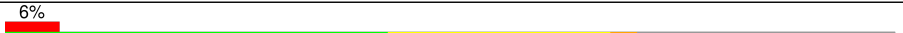



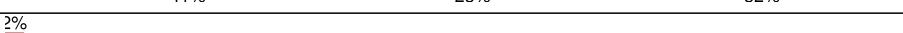









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	110	
1	B	110	
1	G	110	
1	H	110	
1	M	110	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	N	110	
1	S	110	
1	T	110	
1	a	110	
1	b	110	
1	g	110	
1	h	110	
2	C	106	
2	D	106	
2	I	106	
2	J	106	
2	O	106	
2	P	106	
2	U	106	
2	V	106	
2	c	106	
2	d	106	
2	i	106	
2	j	106	
3	E	124	
3	F	124	
3	K	124	
3	L	124	
3	Q	124	
3	R	124	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	W	124	
3	X	124	
3	e	124	
3	f	124	
3	k	124	
3	l	124	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	F	202	X	-	-	-
4	NAG	K	202	X	-	-	-
4	NAG	L	202	X	-	-	-
4	NAG	X	202	X	-	-	-
4	NAG	k	202	X	-	-	-
4	NAG	l	202	X	-	-	-
5	NA	e	203	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25411 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 Growth/differentiation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			821	528	134	150	9			
1	B	105	Total	C	N	O	S	0	0	0
			814	523	133	150	8			
1	G	105	Total	C	N	O	S	0	0	0
			810	520	132	150	8			
1	H	105	Total	C	N	O	S	0	0	0
			821	528	134	150	9			
1	M	105	Total	C	N	O	S	0	0	0
			817	525	133	150	9			
1	N	104	Total	C	N	O	S	0	0	0
			801	515	128	149	9			
1	S	105	Total	C	N	O	S	0	0	0
			821	528	134	150	9			
1	T	105	Total	C	N	O	S	0	0	0
			813	522	132	150	9			
1	a	105	Total	C	N	O	S	0	0	0
			806	518	129	150	9			
1	b	105	Total	C	N	O	S	0	0	0
			821	528	134	150	9			
1	g	105	Total	C	N	O	S	0	0	0
			820	528	133	150	9			
1	h	105	Total	C	N	O	S	0	0	0
			821	528	134	150	9			

- Molecule 2 is a protein called Serine/threonine-protein kinase receptor R3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	0	0	0
			567	344	111	102	10			
2	D	72	Total	C	N	O	S	0	0	0
			553	333	110	100	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	75	Total	C	N	O	S	0	0	0
			556	338	110	98	10			
2	J	72	Total	C	N	O	S	0	0	0
			539	327	104	98	10			
2	O	75	Total	C	N	O	S	0	0	0
			531	325	99	97	10			
2	P	72	Total	C	N	O	S	0	0	0
			549	333	110	96	10			
2	U	75	Total	C	N	O	S	0	0	0
			572	346	112	104	10			
2	V	72	Total	C	N	O	S	0	0	0
			553	333	111	99	10			
2	c	75	Total	C	N	O	S	0	0	0
			561	340	113	98	10			
2	d	72	Total	C	N	O	S	0	0	0
			539	328	104	97	10			
2	i	75	Total	C	N	O	S	0	0	0
			559	339	109	101	10			
2	j	72	Total	C	N	O	S	0	0	0
			559	336	113	100	10			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	EXPRESSION TAG	UNP P37023
C	21	ALA	-	EXPRESSION TAG	UNP P37023
C	119	SER	-	EXPRESSION TAG	UNP P37023
C	120	GLY	-	EXPRESSION TAG	UNP P37023
C	121	ASP	-	EXPRESSION TAG	UNP P37023
C	122	ASP	-	EXPRESSION TAG	UNP P37023
C	123	ASP	-	EXPRESSION TAG	UNP P37023
C	124	ASP	-	EXPRESSION TAG	UNP P37023
C	125	LYS	-	EXPRESSION TAG	UNP P37023
D	20	GLY	-	EXPRESSION TAG	UNP P37023
D	21	ALA	-	EXPRESSION TAG	UNP P37023
D	119	SER	-	EXPRESSION TAG	UNP P37023
D	120	GLY	-	EXPRESSION TAG	UNP P37023
D	121	ASP	-	EXPRESSION TAG	UNP P37023
D	122	ASP	-	EXPRESSION TAG	UNP P37023
D	123	ASP	-	EXPRESSION TAG	UNP P37023
D	124	ASP	-	EXPRESSION TAG	UNP P37023
D	125	LYS	-	EXPRESSION TAG	UNP P37023
I	20	GLY	-	EXPRESSION TAG	UNP P37023

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	21	ALA	-	EXPRESSION TAG	UNP P37023
I	119	SER	-	EXPRESSION TAG	UNP P37023
I	120	GLY	-	EXPRESSION TAG	UNP P37023
I	121	ASP	-	EXPRESSION TAG	UNP P37023
I	122	ASP	-	EXPRESSION TAG	UNP P37023
I	123	ASP	-	EXPRESSION TAG	UNP P37023
I	124	ASP	-	EXPRESSION TAG	UNP P37023
I	125	LYS	-	EXPRESSION TAG	UNP P37023
J	20	GLY	-	EXPRESSION TAG	UNP P37023
J	21	ALA	-	EXPRESSION TAG	UNP P37023
J	119	SER	-	EXPRESSION TAG	UNP P37023
J	120	GLY	-	EXPRESSION TAG	UNP P37023
J	121	ASP	-	EXPRESSION TAG	UNP P37023
J	122	ASP	-	EXPRESSION TAG	UNP P37023
J	123	ASP	-	EXPRESSION TAG	UNP P37023
J	124	ASP	-	EXPRESSION TAG	UNP P37023
J	125	LYS	-	EXPRESSION TAG	UNP P37023
O	20	GLY	-	EXPRESSION TAG	UNP P37023
O	21	ALA	-	EXPRESSION TAG	UNP P37023
O	119	SER	-	EXPRESSION TAG	UNP P37023
O	120	GLY	-	EXPRESSION TAG	UNP P37023
O	121	ASP	-	EXPRESSION TAG	UNP P37023
O	122	ASP	-	EXPRESSION TAG	UNP P37023
O	123	ASP	-	EXPRESSION TAG	UNP P37023
O	124	ASP	-	EXPRESSION TAG	UNP P37023
O	125	LYS	-	EXPRESSION TAG	UNP P37023
P	20	GLY	-	EXPRESSION TAG	UNP P37023
P	21	ALA	-	EXPRESSION TAG	UNP P37023
P	119	SER	-	EXPRESSION TAG	UNP P37023
P	120	GLY	-	EXPRESSION TAG	UNP P37023
P	121	ASP	-	EXPRESSION TAG	UNP P37023
P	122	ASP	-	EXPRESSION TAG	UNP P37023
P	123	ASP	-	EXPRESSION TAG	UNP P37023
P	124	ASP	-	EXPRESSION TAG	UNP P37023
P	125	LYS	-	EXPRESSION TAG	UNP P37023
U	20	GLY	-	EXPRESSION TAG	UNP P37023
U	21	ALA	-	EXPRESSION TAG	UNP P37023
U	119	SER	-	EXPRESSION TAG	UNP P37023
U	120	GLY	-	EXPRESSION TAG	UNP P37023
U	121	ASP	-	EXPRESSION TAG	UNP P37023
U	122	ASP	-	EXPRESSION TAG	UNP P37023
U	123	ASP	-	EXPRESSION TAG	UNP P37023

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	124	ASP	-	EXPRESSION TAG	UNP P37023
U	125	LYS	-	EXPRESSION TAG	UNP P37023
V	20	GLY	-	EXPRESSION TAG	UNP P37023
V	21	ALA	-	EXPRESSION TAG	UNP P37023
V	119	SER	-	EXPRESSION TAG	UNP P37023
V	120	GLY	-	EXPRESSION TAG	UNP P37023
V	121	ASP	-	EXPRESSION TAG	UNP P37023
V	122	ASP	-	EXPRESSION TAG	UNP P37023
V	123	ASP	-	EXPRESSION TAG	UNP P37023
V	124	ASP	-	EXPRESSION TAG	UNP P37023
V	125	LYS	-	EXPRESSION TAG	UNP P37023
c	20	GLY	-	EXPRESSION TAG	UNP P37023
c	21	ALA	-	EXPRESSION TAG	UNP P37023
c	119	SER	-	EXPRESSION TAG	UNP P37023
c	120	GLY	-	EXPRESSION TAG	UNP P37023
c	121	ASP	-	EXPRESSION TAG	UNP P37023
c	122	ASP	-	EXPRESSION TAG	UNP P37023
c	123	ASP	-	EXPRESSION TAG	UNP P37023
c	124	ASP	-	EXPRESSION TAG	UNP P37023
c	125	LYS	-	EXPRESSION TAG	UNP P37023
d	20	GLY	-	EXPRESSION TAG	UNP P37023
d	21	ALA	-	EXPRESSION TAG	UNP P37023
d	119	SER	-	EXPRESSION TAG	UNP P37023
d	120	GLY	-	EXPRESSION TAG	UNP P37023
d	121	ASP	-	EXPRESSION TAG	UNP P37023
d	122	ASP	-	EXPRESSION TAG	UNP P37023
d	123	ASP	-	EXPRESSION TAG	UNP P37023
d	124	ASP	-	EXPRESSION TAG	UNP P37023
d	125	LYS	-	EXPRESSION TAG	UNP P37023
i	20	GLY	-	EXPRESSION TAG	UNP P37023
i	21	ALA	-	EXPRESSION TAG	UNP P37023
i	119	SER	-	EXPRESSION TAG	UNP P37023
i	120	GLY	-	EXPRESSION TAG	UNP P37023
i	121	ASP	-	EXPRESSION TAG	UNP P37023
i	122	ASP	-	EXPRESSION TAG	UNP P37023
i	123	ASP	-	EXPRESSION TAG	UNP P37023
i	124	ASP	-	EXPRESSION TAG	UNP P37023
i	125	LYS	-	EXPRESSION TAG	UNP P37023
j	20	GLY	-	EXPRESSION TAG	UNP P37023
j	21	ALA	-	EXPRESSION TAG	UNP P37023
j	119	SER	-	EXPRESSION TAG	UNP P37023
j	120	GLY	-	EXPRESSION TAG	UNP P37023

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
j	121	ASP	-	EXPRESSION TAG	UNP P37023
j	122	ASP	-	EXPRESSION TAG	UNP P37023
j	123	ASP	-	EXPRESSION TAG	UNP P37023
j	124	ASP	-	EXPRESSION TAG	UNP P37023
j	125	LYS	-	EXPRESSION TAG	UNP P37023

- Molecule 3 is a protein called Activin receptor type-2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	91	Total	C	N	O	S	0	0	0
			739	457	132	140	10			
3	F	91	Total	C	N	O	S	0	0	0
			716	445	127	134	10			
3	K	91	Total	C	N	O	S	0	0	0
			709	441	125	133	10			
3	L	91	Total	C	N	O	S	0	0	0
			725	448	129	138	10			
3	Q	91	Total	C	N	O	S	0	0	0
			736	455	129	142	10			
3	R	91	Total	C	N	O	S	0	0	0
			718	445	126	137	10			
3	W	91	Total	C	N	O	S	0	0	0
			726	449	129	138	10			
3	X	91	Total	C	N	O	S	0	0	0
			711	440	126	135	10			
3	e	91	Total	C	N	O	S	0	0	0
			718	444	123	141	10			
3	f	91	Total	C	N	O	S	0	0	0
			725	448	127	140	10			
3	k	91	Total	C	N	O	S	0	0	0
			710	441	122	137	10			
3	l	91	Total	C	N	O	S	0	0	0
			712	442	125	135	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	EXPRESSION TAG	UNP Q13705
E	0	ALA	-	EXPRESSION TAG	UNP Q13705
E	117	GLY	-	EXPRESSION TAG	UNP Q13705
E	118	ASP	-	EXPRESSION TAG	UNP Q13705
E	119	ASP	-	EXPRESSION TAG	UNP Q13705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	120	ASP	-	EXPRESSION TAG	UNP Q13705
E	121	ASP	-	EXPRESSION TAG	UNP Q13705
E	122	LYS	-	EXPRESSION TAG	UNP Q13705
F	-1	GLY	-	EXPRESSION TAG	UNP Q13705
F	0	ALA	-	EXPRESSION TAG	UNP Q13705
F	117	GLY	-	EXPRESSION TAG	UNP Q13705
F	118	ASP	-	EXPRESSION TAG	UNP Q13705
F	119	ASP	-	EXPRESSION TAG	UNP Q13705
F	120	ASP	-	EXPRESSION TAG	UNP Q13705
F	121	ASP	-	EXPRESSION TAG	UNP Q13705
F	122	LYS	-	EXPRESSION TAG	UNP Q13705
K	-1	GLY	-	EXPRESSION TAG	UNP Q13705
K	0	ALA	-	EXPRESSION TAG	UNP Q13705
K	117	GLY	-	EXPRESSION TAG	UNP Q13705
K	118	ASP	-	EXPRESSION TAG	UNP Q13705
K	119	ASP	-	EXPRESSION TAG	UNP Q13705
K	120	ASP	-	EXPRESSION TAG	UNP Q13705
K	121	ASP	-	EXPRESSION TAG	UNP Q13705
K	122	LYS	-	EXPRESSION TAG	UNP Q13705
L	-1	GLY	-	EXPRESSION TAG	UNP Q13705
L	0	ALA	-	EXPRESSION TAG	UNP Q13705
L	117	GLY	-	EXPRESSION TAG	UNP Q13705
L	118	ASP	-	EXPRESSION TAG	UNP Q13705
L	119	ASP	-	EXPRESSION TAG	UNP Q13705
L	120	ASP	-	EXPRESSION TAG	UNP Q13705
L	121	ASP	-	EXPRESSION TAG	UNP Q13705
L	122	LYS	-	EXPRESSION TAG	UNP Q13705
Q	-1	GLY	-	EXPRESSION TAG	UNP Q13705
Q	0	ALA	-	EXPRESSION TAG	UNP Q13705
Q	117	GLY	-	EXPRESSION TAG	UNP Q13705
Q	118	ASP	-	EXPRESSION TAG	UNP Q13705
Q	119	ASP	-	EXPRESSION TAG	UNP Q13705
Q	120	ASP	-	EXPRESSION TAG	UNP Q13705
Q	121	ASP	-	EXPRESSION TAG	UNP Q13705
Q	122	LYS	-	EXPRESSION TAG	UNP Q13705
R	-1	GLY	-	EXPRESSION TAG	UNP Q13705
R	0	ALA	-	EXPRESSION TAG	UNP Q13705
R	117	GLY	-	EXPRESSION TAG	UNP Q13705
R	118	ASP	-	EXPRESSION TAG	UNP Q13705
R	119	ASP	-	EXPRESSION TAG	UNP Q13705
R	120	ASP	-	EXPRESSION TAG	UNP Q13705
R	121	ASP	-	EXPRESSION TAG	UNP Q13705

Continued on next page...

Continued from previous page...

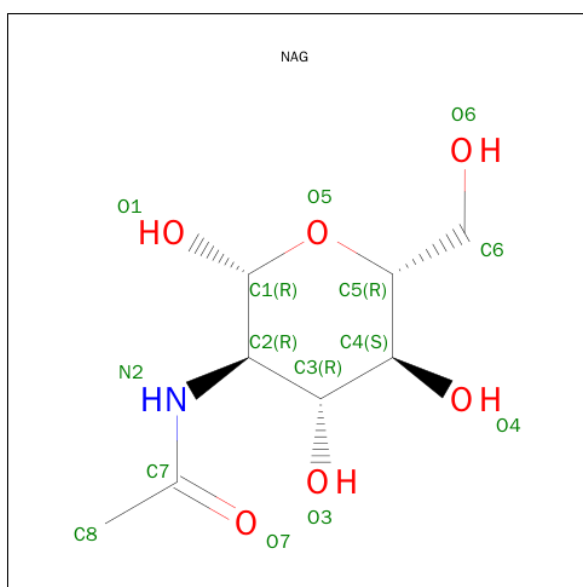
Chain	Residue	Modelled	Actual	Comment	Reference
R	122	LYS	-	EXPRESSION TAG	UNP Q13705
W	-1	GLY	-	EXPRESSION TAG	UNP Q13705
W	0	ALA	-	EXPRESSION TAG	UNP Q13705
W	117	GLY	-	EXPRESSION TAG	UNP Q13705
W	118	ASP	-	EXPRESSION TAG	UNP Q13705
W	119	ASP	-	EXPRESSION TAG	UNP Q13705
W	120	ASP	-	EXPRESSION TAG	UNP Q13705
W	121	ASP	-	EXPRESSION TAG	UNP Q13705
W	122	LYS	-	EXPRESSION TAG	UNP Q13705
X	-1	GLY	-	EXPRESSION TAG	UNP Q13705
X	0	ALA	-	EXPRESSION TAG	UNP Q13705
X	117	GLY	-	EXPRESSION TAG	UNP Q13705
X	118	ASP	-	EXPRESSION TAG	UNP Q13705
X	119	ASP	-	EXPRESSION TAG	UNP Q13705
X	120	ASP	-	EXPRESSION TAG	UNP Q13705
X	121	ASP	-	EXPRESSION TAG	UNP Q13705
X	122	LYS	-	EXPRESSION TAG	UNP Q13705
e	-1	GLY	-	EXPRESSION TAG	UNP Q13705
e	0	ALA	-	EXPRESSION TAG	UNP Q13705
e	117	GLY	-	EXPRESSION TAG	UNP Q13705
e	118	ASP	-	EXPRESSION TAG	UNP Q13705
e	119	ASP	-	EXPRESSION TAG	UNP Q13705
e	120	ASP	-	EXPRESSION TAG	UNP Q13705
e	121	ASP	-	EXPRESSION TAG	UNP Q13705
e	122	LYS	-	EXPRESSION TAG	UNP Q13705
f	-1	GLY	-	EXPRESSION TAG	UNP Q13705
f	0	ALA	-	EXPRESSION TAG	UNP Q13705
f	117	GLY	-	EXPRESSION TAG	UNP Q13705
f	118	ASP	-	EXPRESSION TAG	UNP Q13705
f	119	ASP	-	EXPRESSION TAG	UNP Q13705
f	120	ASP	-	EXPRESSION TAG	UNP Q13705
f	121	ASP	-	EXPRESSION TAG	UNP Q13705
f	122	LYS	-	EXPRESSION TAG	UNP Q13705
k	-1	GLY	-	EXPRESSION TAG	UNP Q13705
k	0	ALA	-	EXPRESSION TAG	UNP Q13705
k	117	GLY	-	EXPRESSION TAG	UNP Q13705
k	118	ASP	-	EXPRESSION TAG	UNP Q13705
k	119	ASP	-	EXPRESSION TAG	UNP Q13705
k	120	ASP	-	EXPRESSION TAG	UNP Q13705
k	121	ASP	-	EXPRESSION TAG	UNP Q13705
k	122	LYS	-	EXPRESSION TAG	UNP Q13705
l	-1	GLY	-	EXPRESSION TAG	UNP Q13705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	EXPRESSION TAG	UNP Q13705
1	117	GLY	-	EXPRESSION TAG	UNP Q13705
1	118	ASP	-	EXPRESSION TAG	UNP Q13705
1	119	ASP	-	EXPRESSION TAG	UNP Q13705
1	120	ASP	-	EXPRESSION TAG	UNP Q13705
1	121	ASP	-	EXPRESSION TAG	UNP Q13705
1	122	LYS	-	EXPRESSION TAG	UNP Q13705

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	e	1	Total	C	N	O	0	0
			14	8	1	5		
4	e	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	k	1	Total	C	N	O	0	0
			14	8	1	5		
4	k	1	Total	C	N	O	0	0
			14	8	1	5		
4	l	1	Total	C	N	O	0	0
			14	8	1	5		
4	l	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

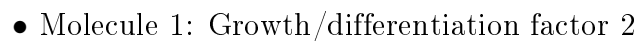
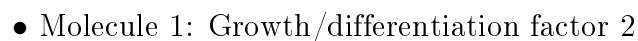
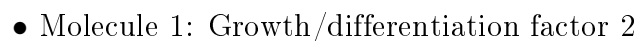
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	k	1	Total	Na	0	0
			1	1		
5	e	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	1	Total 1	Na 1	0	0
5	R	1	Total 1	Na 1	0	0
5	F	1	Total 1	Na 1	0	0
5	K	1	Total 1	Na 1	0	0

- Molecule 1: Growth/differentiation factor 2



-
- SER
ALA
GLY
ALA
GLY
S6
T50
D88
K96
Y97
H98
R110

- Molecule 1: Growth/differentiation factor 2

Chain g:  92% 5%



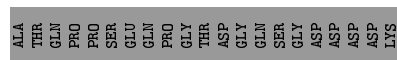
- Molecule 1: Growth/differentiation factor 2

Chain h:  92% 5%

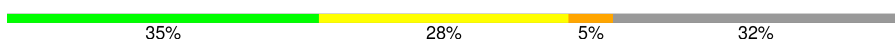


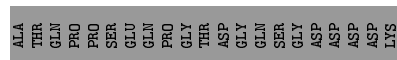
- Molecule 2: Serine/threonine-protein kinase receptor R3

Chain C:  41% 27% 29%



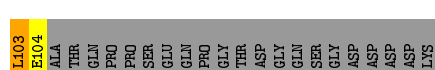
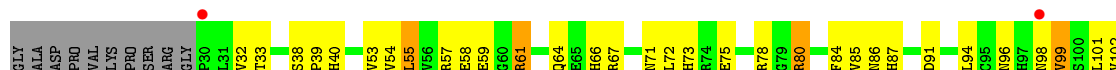
- Molecule 2: Serine/threonine-protein kinase receptor R3

Chain D:  35% 28% 5% 32%



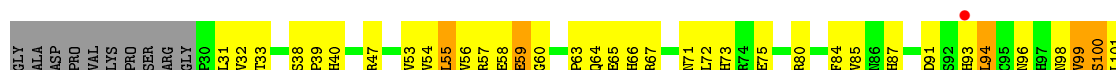
- Molecule 2: Serine/threonine-protein kinase receptor R3

Chain I:  2% 39% 27% 5% 29%



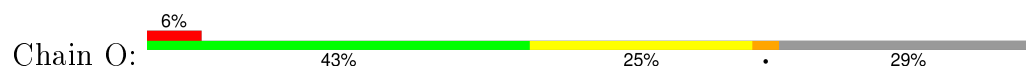
- Molecule 2: Serine/threonine-protein kinase receptor R3

Chain J:  34% 29% 5% 32%



VAL
LEU
GLU
ALA
THR
GLN
PRO
SER
PRO
GLN
GLY
THR
ASP
GLY
GLN
SER
GLY
ASP
ASP
ASP
LYS

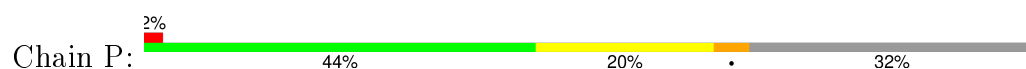
• Molecule 2: Serine/threonine-protein kinase receptor R3



GLY
ALA
PRO
VAL
LYS
PRO
SER
ARG
GLY
P30
L31
V32
T33
P44
G48
A49
V53
V54
L55
V56
R57
E58
E59
G60
R61
H62
P63
H66
R67
N71
L72
H73
R80
E83
F84
V85
H86
H87
D81
S92
H93
L94
C95
N96
H97
N98
V99
V102
L103
E104

ALA
THR
GLN
PRO
VAL
LYS
PRO
SER
GLU
GLN
PRO
SER
GLY
THR
ASP
GLY
GLN
GLN
SER
GLY
ASP
ASP
LYS

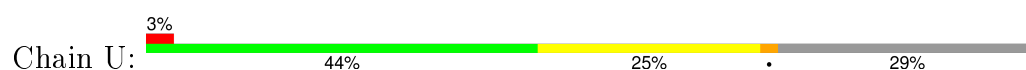
• Molecule 2: Serine/threonine-protein kinase receptor R3



GLY
ALA
PRO
VAL
LYS
PRO
SER
ARG
GLY
P30
L31
V32
T33
V53
V54
L55
E59
Q64
E65
H66
R67
N71
L72
H73
R74
E75
L76
R80
F84
V85
H86
H87
D91
S92
H93
L94
N98
V99
S100
L101
VAL
LEU
GLU
ALA
THR
PRO
GLN

PRO
GLY
THR
ASP
GLY
GLN
SER
GLY
THR
ASP
ASP
LYS

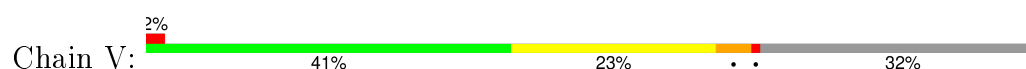
• Molecule 2: Serine/threonine-protein kinase receptor R3



GLY
ALA
PRO
VAL
LYS
PRO
SER
ARG
GLY
P30
L31
V32
T33
S38
P39
V53
V54
L55
E58
E59
G60
R61
H62
P63
Q64
E65
H66
R67
N71
L72
H73
R74
E75
R80
F84
V85
H86
H87
D91
L94
N98
V99
S100
L101
V102
L103
E104
ALA
THR
GLN

PRO
PRO
SER
GLU
GLN
PRO
GLY
THR
GLY
GLY
SER
GLY
ASP
ASP
ASP
LYS

• Molecule 2: Serine/threonine-protein kinase receptor R3



GLY
ALA
PRO
VAL
LYS
PRO
SER
ARG
GLY
P30
L31
V32
T33
S38
P39
V53
V54
L55
E58
E59
G60
R61
Q64
E65
H66
R67
N71
L72
H73
R74
E75
R80
F84
V85
H86
H87
D91
S92
H93
L94
C95
N96
H97
N98
V99
S100
L101
VAL
LEU
GLU
ALA

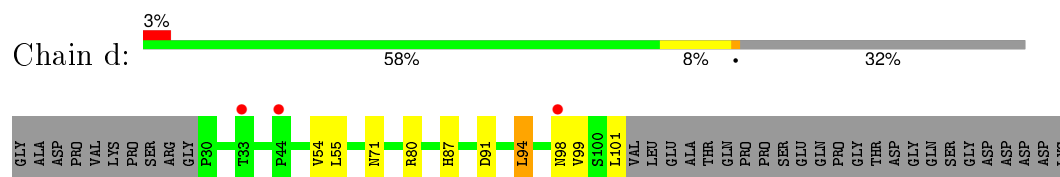
THR
GLN
PRO
PRO
SER
GLU
GLN
PRO
SER
GLY
THR
ASP
GLY
GLN
GLN
SER
GLY
ASP
ASP
ASP
LYS

• Molecule 2: Serine/threonine-protein kinase receptor R3

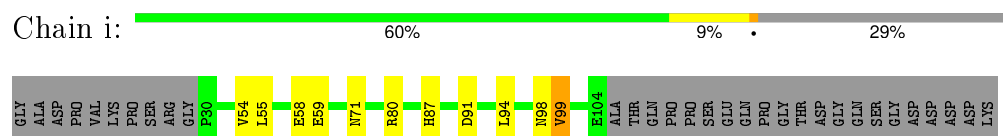


GLY
ALA
PRO
VAL
LYS
PRO
SER
ARG
GLY
P30
V54
L55
E58
N71
R80
H87
D91
L94
H97
N98
V99
E104
ALA
THR
GLN
PRO
PRO
SER
GLU
GLN
GLN
PRO
GLY
THR
ASP
GLY
GLN
SER
GLY
GLY
ASP
ASP
ASP
LYS

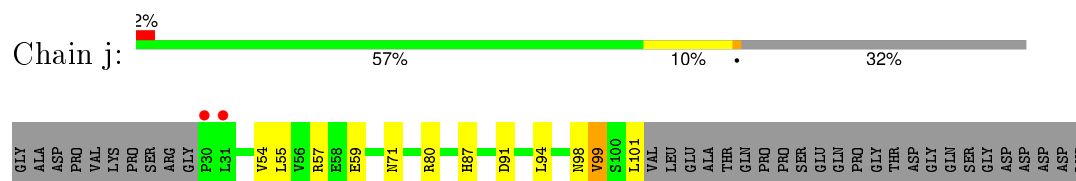
- Molecule 2: Serine/threonine-protein kinase receptor R3



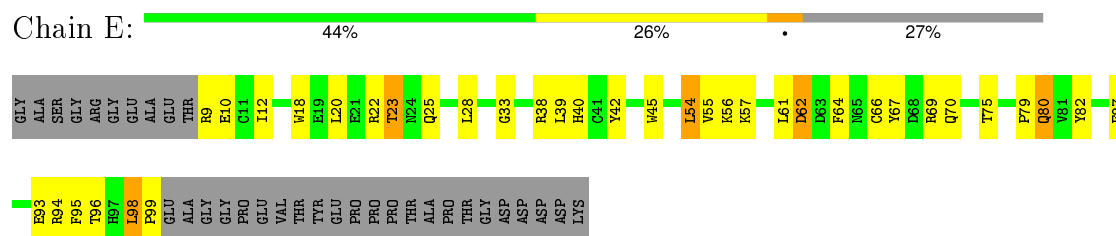
- Molecule 2: Serine/threonine-protein kinase receptor R3



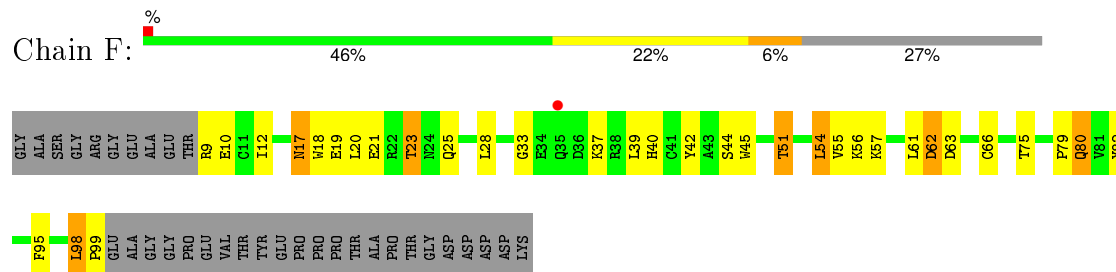
- Molecule 2: Serine/threonine-protein kinase receptor R3



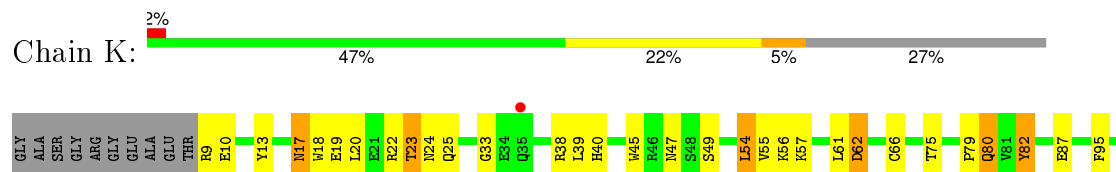
- Molecule 3: Activin receptor type-2B

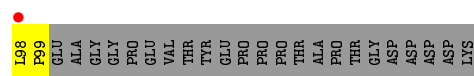


- Molecule 3: Activin receptor type-2B

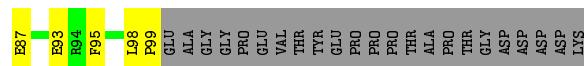
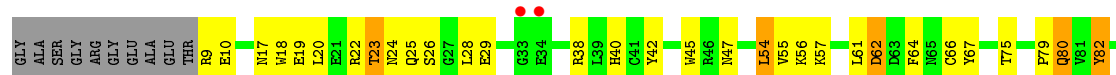


- Molecule 3: Activin receptor type-2B

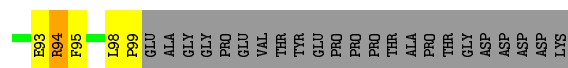
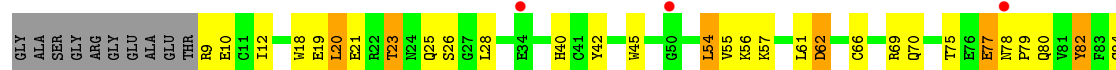
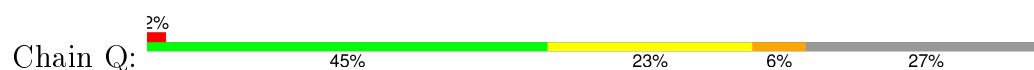




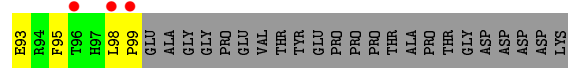
• Molecule 3: Activin receptor type-2B



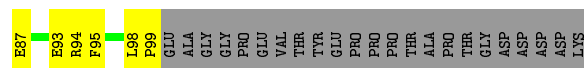
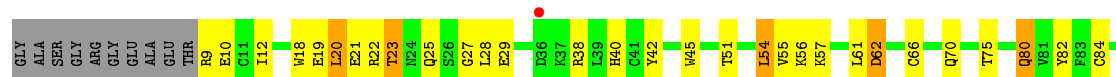
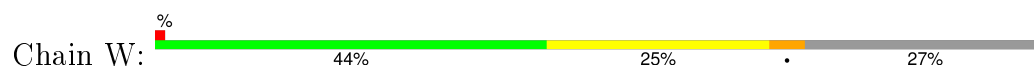
• Molecule 3: Activin receptor type-2B



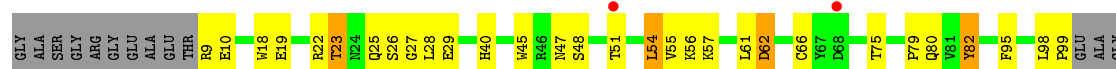
• Molecule 3: Activin receptor type-2B



• Molecule 3: Activin receptor type-2B



• Molecule 3: Activin receptor type-2B



GLY
PRO
GLU
VAL
THR
GLY
GLU
PRO
PRO
THR
ALA
PRO
THR
GLY
ASP
ASP
ASP
LYS

• Molecule 3: Activin receptor type-2B

Chain e:  69% 5% 27%

GLY
ALA
SER
GLY
ARG
GLY
GLU
ALA
GLU
THR
R9
T23
L54
D62
Q80
Y81
Y82
L98
P99
GLU
ALA
GLY
GLY
PRO
GLU
VAL
THR
TYR
GLU
PRO
PRO
GLU
VAL
THR
ALA
GLU
PRO
THR
GLY
ASP
ASP
ASP
LYS

• Molecule 3: Activin receptor type-2B

Chain f:  67% 6% 27%

GLY
ALA
SER
GLY
ARG
GLY
GLU
ALA
GLU
THR
R9
T23
Q35
L54
D62
D63
Q80
Y81
Y82
F83
C84
L98
P99
GLU
ALA
GLY
GLY
PRO
GLU
VAL
THR
TYR
GLU
PRO
PRO
THR
ALA
GLU
PRO
THR
GLY
ASP
ASP
ASP
LYS

• Molecule 3: Activin receptor type-2B

Chain k:  67% 6% 27%

GLY
ALA
SER
GLY
ARG
GLY
GLU
ALA
GLU
THR
R9
M17
T23
G33
T51
L54
D62
Q80
Y81
Y82
T96
H97
L98
P99
GLU
ALA
GLY
GLY
PRO
GLU
VAL
THR
TYR
GLU
PRO
PRO
THR
ALA
GLU
PRO
THR
GLY
ASP
ASP
ASP
LYS

• Molecule 3: Activin receptor type-2B

Chain l:  66% 7% 27%

GLY
ALA
SER
GLY
ARG
GLY
GLU
ALA
GLU
THR
R9
T23
S26
Q35
L54
D62
T75
Q80
Y81
Y82
F83
C84
L98
P99
GLU
ALA
GLY
GLY
PRO
GLU
VAL
THR
TYR
GLU
PRO
PRO
THR
ALA
GLU
PRO
THR
GLY
ASP
ASP
ASP
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	216.45Å 216.45Å 216.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.85 – 3.36 26.85 – 3.36	Depositor EDS
% Data completeness (in resolution range)	84.0 (26.85-3.36) 83.0 (26.85-3.36)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 3.38Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.261 0.208 , 0.250	Depositor DCC
R_{free} test set	1682 reflections (2.42%)	DCC
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.7	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 82408 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25411	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAG

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	0.56	0/844	0.63	0/1144
1	B	0.54	0/837	0.64	0/1137
1	G	0.54	0/833	0.65	0/1133
1	H	0.53	0/844	0.63	0/1144
1	M	0.56	0/840	0.62	0/1140
1	N	0.54	0/823	0.64	0/1119
1	S	0.56	0/844	0.62	0/1144
1	T	0.54	0/836	0.64	0/1136
1	a	0.53	0/828	0.65	0/1126
1	b	0.55	0/844	0.62	0/1144
1	g	0.54	0/843	0.63	0/1142
1	h	0.53	0/844	0.62	0/1144
2	C	0.48	0/582	0.60	0/792
2	D	0.45	0/568	0.64	0/772
2	I	0.46	0/571	0.60	0/778
2	J	0.41	0/553	0.63	0/753
2	O	0.38	0/545	0.57	0/748
2	P	0.41	0/564	0.61	0/767
2	U	0.46	0/587	0.60	0/798
2	V	0.44	0/567	0.65	0/770
2	c	0.40	0/576	0.58	0/785
2	d	0.40	0/554	0.61	0/755
2	i	0.40	0/573	0.60	0/780
2	j	0.40	0/574	0.60	0/779
3	E	0.54	0/757	0.60	0/1024
3	F	0.46	0/734	0.57	0/996
3	K	0.50	0/727	0.61	0/988
3	L	0.52	0/743	0.58	0/1008
3	Q	0.54	0/754	0.59	0/1021
3	R	0.56	0/736	0.60	0/1000
3	W	0.53	0/744	0.60	0/1009
3	X	0.44	0/729	0.57	0/990

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.47	0/736	0.58	0/1000
3	f	0.48	0/743	0.58	0/1008
3	k	0.47	0/728	0.57	0/990
3	l	0.51	0/730	0.58	0/992
All	All	0.50	0/25735	0.61	0/34956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	821	0	801	47	0
1	B	814	0	783	53	0
1	G	810	0	772	50	0
1	H	821	0	801	49	0
1	M	817	0	790	40	0
1	N	801	0	765	47	0
1	S	821	0	801	38	0
1	T	813	0	779	40	0
1	a	806	0	767	0	0
1	b	821	0	801	0	0
1	g	820	0	800	0	0
1	h	821	0	801	0	0
2	C	567	0	509	28	0
2	D	553	0	499	36	0
2	I	556	0	483	31	0
2	J	539	0	478	32	0
2	O	531	0	449	22	0
2	P	549	0	493	18	0
2	U	572	0	514	14	0
2	V	553	0	502	20	0
2	c	561	0	501	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	539	0	476	0	0
2	i	559	0	503	0	0
2	j	559	0	510	0	0
3	E	739	0	637	37	0
3	F	716	0	614	27	0
3	K	709	0	599	24	0
3	L	725	0	620	27	0
3	Q	736	0	634	34	0
3	R	718	0	606	21	0
3	W	726	0	622	33	0
3	X	711	0	599	21	0
3	e	718	0	596	0	0
3	f	725	0	619	0	0
3	k	710	0	594	0	0
3	l	712	0	601	0	0
4	E	28	0	26	0	0
4	F	28	0	26	0	0
4	K	28	0	26	6	0
4	L	28	0	26	3	0
4	Q	28	0	26	1	0
4	R	28	0	26	0	0
4	W	28	0	26	1	0
4	X	28	0	26	7	0
4	e	28	0	26	0	0
4	f	28	0	26	0	0
4	k	28	0	26	0	0
4	l	28	0	26	0	0
5	F	1	0	0	0	0
5	K	1	0	0	0	0
5	R	1	0	0	0	0
5	X	1	0	0	0	0
5	e	1	0	0	0	0
5	k	1	0	0	0	0
All	All	25411	0	23031	669	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 (669) 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:J:100:SER:O	2:J:101:LEU:HD23	1.62	0.99
1:M:64:LYS:HB2	2:P:84:PHE:CE1	2.00	0.97
1:N:35:TYR:HB2	1:N:104:VAL:HB	1.50	0.93
2:U:55:LEU:HD13	2:U:103:LEU:HD13	1.52	0.92
2:D:57:ARG:HD3	2:D:63:PRO:HD3	1.52	0.91
1:A:35:TYR:HB2	1:A:104:VAL:HB	1.53	0.91
1:B:35:TYR:HB2	1:B:104:VAL:HB	1.51	0.90
4:K:201:NAG:H61	4:X:201:NAG:H82	112.46	0.90
2:D:58:GLU:HB3	2:D:59:GLU:HG2	1.54	0.90
3:Q:70:GLN:HG2	1:T:71:LYS:HE3	1.53	0.89
1:G:35:TYR:HB2	1:G:104:VAL:HB	1.52	0.89
1:H:35:TYR:HB2	1:H:104:VAL:HB	1.54	0.89
1:M:35:TYR:HB2	1:M:104:VAL:HB	1.55	0.88
1:T:35:TYR:HB2	1:T:104:VAL:HB	1.56	0.87
2:U:55:LEU:HD13	2:U:103:LEU:CD1	2.05	0.87
1:S:35:TYR:HB2	1:S:104:VAL:HB	1.56	0.86
3:E:54:LEU:HD11	3:E:57:LYS:HE3	1.67	0.86
3:Q:70:GLN:HG2	1:T:71:LYS:CE	2.05	0.86
1:M:75:VAL:HG11	1:N:75:VAL:HG11	1.55	0.86
1:A:75:VAL:HG11	1:B:75:VAL:HG11	1.67	0.86
2:D:57:ARG:HG3	2:D:57:ARG:HH11	1.39	0.85
3:E:93:GLU:OE2	1:H:68:LYS:HD3	1.77	0.85
3:E:69:ARG:HH12	2:I:61:ARG:NH1	1.75	0.84
2:J:57:ARG:HH11	2:J:57:ARG:HG2	2.82	0.84
2:D:57:ARG:HB2	1:S:90:MET:HE1	41.46	0.83
2:C:55:LEU:HD13	2:C:103:LEU:CD1	2.50	0.82
1:M:7:HIS:O	1:M:39:GLY:HA3	1.79	0.82
2:D:93:HIS:CE1	2:D:94:LEU:HD12	2.92	0.82
1:B:71:LYS:CE	3:W:70:GLN:HG2	2.09	0.81
3:E:70:GLN:HG2	1:G:71:LYS:HE3	1.62	0.81
3:F:54:LEU:HD11	3:F:57:LYS:HE3	1.62	0.81
3:R:54:LEU:HD11	3:R:57:LYS:HE3	1.64	0.80
1:B:71:LYS:HE3	3:W:70:GLN:HG2	1.62	0.80
3:Q:54:LEU:HD11	3:Q:57:LYS:HE3	1.63	0.80
1:G:7:HIS:O	1:G:39:GLY:HA3	1.82	0.80
2:O:55:LEU:HD13	2:O:103:LEU:CD1	2.11	0.79
1:B:64:LYS:HB2	2:D:84:PHE:CE1	40.70	0.79
1:A:64:LYS:HB2	2:C:84:PHE:CE1	40.74	0.79
1:B:7:HIS:O	1:B:39:GLY:HA3	1.83	0.79
2:I:55:LEU:HD13	2:I:103:LEU:HD22	3.35	0.79
1:H:7:HIS:O	1:H:39:GLY:HA3	1.84	0.78
3:L:54:LEU:HD11	3:L:57:LYS:HE3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:54:LEU:HD11	3:K:57:LYS:HE3	1.74	0.78
1:S:75:VAL:HG11	1:T:75:VAL:HG11	1.66	0.77
2:J:57:ARG:HH11	2:J:57:ARG:CG	3.13	0.77
1:G:75:VAL:HG11	1:H:75:VAL:HG11	1.67	0.75
3:Q:70:GLN:HG3	1:T:71:LYS:HD2	1.70	0.73
3:W:54:LEU:HD11	3:W:57:LYS:HE3	1.69	0.73
1:S:64:LYS:HB2	2:V:84:PHE:CE1	2.23	0.73
3:E:70:GLN:HG2	1:G:71:LYS:CE	2.19	0.72
3:X:54:LEU:HD11	3:X:57:LYS:HE3	1.73	0.70
2:I:53:VAL:HG12	2:I:101:LEU:HD11	3.20	0.70
2:C:55:LEU:HD13	2:C:103:LEU:HD13	1.71	0.70
1:H:46:ALA:HB2	2:J:40:HIS:ND1	2.08	0.70
1:S:96:LYS:HE3	1:S:98:HIS:H	1.57	0.69
1:S:7:HIS:O	1:S:39:GLY:HA3	1.92	0.69
1:M:96:LYS:HE3	1:M:98:HIS:H	1.57	0.69
1:N:63:LEU:HD23	2:O:58:GLU:HG3	1.73	0.69
1:B:96:LYS:HE3	1:B:98:HIS:H	1.57	0.68
2:D:93:HIS:HE1	2:D:94:LEU:HD12	2.29	0.67
2:D:57:ARG:NH1	2:D:57:ARG:HG3	2.04	0.67
3:R:40:HIS:ND1	3:R:66:CYS:HB2	2.10	0.67
1:G:96:LYS:HE3	1:G:98:HIS:H	1.58	0.67
2:O:55:LEU:HD13	2:O:103:LEU:HD13	1.77	0.67
1:H:53:LYS:HE3	2:J:75:GLU:OE2	2.12	0.67
1:A:96:LYS:HE3	1:A:98:HIS:H	1.60	0.66
3:Q:12:ILE:HD11	1:S:67:THR:HB	1.75	0.66
1:H:64:LYS:HB2	2:J:84:PHE:CE1	2.45	0.66
2:D:57:ARG:HB2	1:S:90:MET:CE	41.54	0.66
1:M:64:LYS:CB	2:P:84:PHE:CE1	2.78	0.66
1:N:63:LEU:CD2	2:O:58:GLU:HG3	2.27	0.65
1:B:71:LYS:HD2	3:W:70:GLN:HG3	1.76	0.65
3:L:40:HIS:ND1	3:L:66:CYS:HB2	2.11	0.65
1:T:96:LYS:HE3	1:T:98:HIS:H	1.61	0.65
1:N:7:HIS:O	1:N:39:GLY:HA3	1.97	0.64
1:H:53:LYS:NZ	2:J:73:HIS:ND1	2.39	0.64
1:N:96:LYS:HE3	1:N:98:HIS:H	1.62	0.64
2:D:57:ARG:HD3	2:D:63:PRO:CD	2.27	0.64
1:N:64:LYS:HB2	2:O:84:PHE:CE1	2.33	0.64
3:L:29:GLU:HG3	4:W:201:NAG:H3	87.93	0.64
3:F:40:HIS:ND1	3:F:66:CYS:HB2	2.19	0.64
1:B:62:HIS:HD2	1:B:69:VAL:O	1.80	0.63
1:H:62:HIS:HD2	1:H:69:VAL:O	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:VAL:HG12	2:C:101:LEU:HD12	1.80	0.62
1:B:53:LYS:HE3	2:D:75:GLU:OE2	36.19	0.62
2:V:59:GLU:O	2:V:61:ARG:N	2.27	0.62
1:M:64:LYS:HB2	2:P:84:PHE:CZ	2.34	0.62
3:Q:94:ARG:HD2	1:T:38:LYS:HD3	1.80	0.62
1:T:7:HIS:O	1:T:39:GLY:HA3	2.00	0.62
1:G:62:HIS:HD2	1:G:69:VAL:O	1.82	0.62
4:K:201:NAG:C6	4:X:201:NAG:H82	113.31	0.62
1:H:96:LYS:HE3	1:H:98:HIS:H	1.64	0.62
3:K:55:VAL:O	3:K:56:LYS:HG3	2.03	0.62
1:A:62:HIS:HD2	1:A:69:VAL:O	1.87	0.61
2:V:100:SER:C	2:V:101:LEU:HD23	2.20	0.61
1:M:53:LYS:HE3	2:P:75:GLU:OE2	2.01	0.61
1:B:80:SER:OG	3:F:37:LYS:HE3	2.01	0.61
3:E:40:HIS:ND1	3:E:66:CYS:HB2	2.21	0.61
1:B:64:LYS:HB2	2:C:84:PHE:CE1	2.36	0.60
1:A:66:PRO:HD2	3:L:19:GLU:HB3	82.72	0.60
2:I:104:GLU:HA	2:I:104:GLU:OE1	2.01	0.60
1:T:62:HIS:HD2	1:T:69:VAL:O	1.84	0.60
3:K:40:HIS:ND1	3:K:66:CYS:HB2	2.21	0.60
1:A:53:LYS:HE3	2:D:75:GLU:OE2	2.01	0.60
1:H:65:PHE:N	1:H:66:PRO:HD3	2.17	0.60
1:M:75:VAL:CG1	1:N:75:VAL:HG11	2.27	0.59
1:B:65:PHE:CD2	3:W:19:GLU:OE1	48.96	0.59
1:N:62:HIS:HD2	1:N:69:VAL:O	1.85	0.59
3:E:55:VAL:O	3:E:56:LYS:HG3	2.08	0.59
2:V:93:HIS:CE1	2:V:94:LEU:HD12	2.38	0.58
1:G:7:HIS:O	1:G:39:GLY:CA	2.50	0.58
1:S:50:THR:HB	1:S:110:ARG:HH22	1.69	0.58
1:A:85:LEU:HD12	1:A:94:THR:O	2.14	0.58
3:E:18:TRP:CD1	3:E:25:GLN:HG3	2.38	0.58
2:I:55:LEU:HD13	2:I:103:LEU:CD2	2.42	0.58
2:J:31:LEU:HB2	2:J:47:ARG:HH21	1.68	0.58
1:A:75:VAL:HG11	1:B:75:VAL:CG1	2.47	0.57
1:S:62:HIS:HD2	1:S:69:VAL:O	1.88	0.57
4:L:202:NAG:H3	4:L:202:NAG:O7	2.03	0.57
2:D:65:GLU:OE2	2:D:101:LEU:HD12	2.05	0.57
3:X:40:HIS:ND1	3:X:66:CYS:HB2	2.19	0.57
1:A:68:LYS:HD3	3:W:93:GLU:OE2	2.05	0.57
2:J:100:SER:C	2:J:101:LEU:HG	2.76	0.56
1:A:64:LYS:HB2	2:D:84:PHE:CE1	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:VAL:HG11	1:M:109:CYS:SG	2.45	0.56
2:J:58:GLU:HG3	2:J:59:GLU:H	2.82	0.56
3:F:45:TRP:CD2	3:F:95:PHE:CE1	2.93	0.56
1:H:50:THR:HB	1:H:110:ARG:HH22	1.71	0.56
1:A:49:VAL:HG12	1:A:49:VAL:O	2.08	0.56
1:H:49:VAL:O	1:H:49:VAL:HG12	2.09	0.56
1:A:67:THR:HB	3:W:12:ILE:HD11	1.88	0.56
2:C:57:ARG:HG3	2:C:63:PRO:HD3	2.25	0.56
3:W:55:VAL:O	3:W:56:LYS:HG3	2.06	0.56
3:E:70:GLN:HG3	1:G:71:LYS:HD2	1.88	0.55
1:G:66:PRO:CG	2:I:59:GLU:HB3	4.60	0.55
3:W:40:HIS:ND1	3:W:66:CYS:HB2	2.20	0.55
1:B:50:THR:HB	1:B:110:ARG:HH22	1.73	0.55
1:B:7:HIS:O	1:B:39:GLY:CA	2.52	0.55
3:Q:93:GLU:OE2	1:S:68:LYS:HD3	2.06	0.55
2:I:57:ARG:O	2:I:59:GLU:N	3.76	0.55
3:R:55:VAL:O	3:R:56:LYS:HG3	2.05	0.55
2:C:55:LEU:HD13	2:C:103:LEU:HD12	2.97	0.55
1:M:75:VAL:HG11	1:N:75:VAL:CG1	2.32	0.55
3:Q:40:HIS:ND1	3:Q:66:CYS:HB2	2.21	0.55
1:T:49:VAL:O	1:T:49:VAL:HG12	2.07	0.55
1:N:49:VAL:HG12	1:N:49:VAL:O	2.07	0.55
1:S:65:PHE:N	1:S:66:PRO:HD3	2.21	0.55
1:A:92:VAL:O	1:A:94:THR:HG23	2.10	0.55
1:N:49:VAL:HG11	1:N:109:CYS:SG	2.47	0.55
1:A:75:VAL:CG1	1:B:75:VAL:HG11	2.41	0.54
3:K:18:TRP:HB2	3:K:23:THR:O	2.07	0.54
3:E:18:TRP:HB2	3:E:23:THR:O	2.07	0.54
1:M:49:VAL:O	1:M:49:VAL:HG12	2.06	0.54
3:E:12:ILE:HD11	1:H:67:THR:HB	1.89	0.54
1:M:62:HIS:HD2	1:M:69:VAL:O	1.90	0.54
3:K:49:SER:HA	4:K:202:NAG:O7	2.26	0.54
3:K:45:TRP:CD2	3:K:95:PHE:CE1	2.96	0.54
2:J:38:SER:OG	2:J:39:PRO:HD2	2.09	0.54
2:D:55:LEU:HD13	1:S:90:MET:HG2	50.69	0.54
1:H:7:HIS:O	1:H:39:GLY:CA	2.58	0.54
1:B:53:LYS:HE3	2:C:75:GLU:OE2	2.08	0.54
2:D:38:SER:OG	2:D:39:PRO:HD2	2.10	0.54
1:T:64:LYS:HB2	2:U:84:PHE:CE1	2.42	0.54
2:J:100:SER:C	2:J:101:LEU:HD23	2.28	0.54
1:H:46:ALA:HB2	2:J:40:HIS:CE1	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:VAL:O	1:H:49:VAL:CG1	2.59	0.54
1:M:95:LEU:HD22	3:Q:42:TYR:CZ	2.43	0.54
1:B:49:VAL:O	1:B:49:VAL:HG12	2.08	0.53
3:X:55:VAL:O	3:X:56:LYS:HG3	2.08	0.53
2:J:65:GLU:OE2	2:J:101:LEU:HD12	4.67	0.53
3:Q:70:GLN:CG	1:T:71:LYS:HD2	2.38	0.53
3:Q:45:TRP:CD2	3:Q:95:PHE:CE1	2.96	0.53
1:G:85:LEU:HD12	1:G:94:THR:O	2.15	0.53
3:R:79:PRO:HD2	3:R:82:TYR:CE2	2.44	0.53
3:W:45:TRP:CD2	3:W:95:PHE:CE1	2.97	0.53
1:S:95:LEU:HD22	3:W:42:TYR:CZ	2.42	0.53
1:G:65:PHE:N	1:G:66:PRO:HD3	2.24	0.53
2:C:86:ASN:ND2	2:C:101:LEU:HD22	2.23	0.53
3:Q:77:GLU:HG3	3:Q:78:ASN:N	2.23	0.53
3:R:45:TRP:CD2	3:R:95:PHE:CE1	2.95	0.53
1:H:49:VAL:HG11	1:H:109:CYS:SG	2.55	0.53
1:S:53:LYS:HE3	2:V:75:GLU:OE2	2.09	0.53
3:W:18:TRP:HB2	3:W:23:THR:O	2.08	0.53
3:R:18:TRP:HB2	3:R:23:THR:O	2.08	0.53
1:H:85:LEU:HD12	1:H:94:THR:O	2.09	0.53
3:K:13:TYR:CE2	4:X:201:NAG:H62	121.13	0.53
2:D:57:ARG:CG	2:D:57:ARG:HH11	2.16	0.53
1:H:71:LYS:NZ	2:J:59:GLU:OE2	2.35	0.53
2:C:32:VAL:HG22	2:C:33:THR:N	2.24	0.53
3:F:18:TRP:HB2	3:F:23:THR:O	2.09	0.53
1:S:49:VAL:HG11	1:S:109:CYS:SG	2.49	0.52
2:V:100:SER:O	2:V:101:LEU:HD23	2.10	0.52
1:B:49:VAL:O	1:B:49:VAL:CG1	2.57	0.52
3:R:40:HIS:CE1	3:R:66:CYS:HB2	2.44	0.52
3:L:40:HIS:CE1	3:L:66:CYS:HB2	2.44	0.52
1:G:64:LYS:HB2	2:I:84:PHE:CE1	2.45	0.52
3:F:79:PRO:HD2	3:F:82:TYR:CE2	2.56	0.52
3:Q:18:TRP:HB2	3:Q:23:THR:O	2.10	0.52
2:P:32:VAL:HG22	2:P:33:THR:N	2.25	0.52
2:I:86:ASN:ND2	2:I:101:LEU:HD22	2.25	0.52
1:G:49:VAL:HG12	1:G:49:VAL:O	2.08	0.52
2:V:32:VAL:HG22	2:V:33:THR:N	2.25	0.52
1:B:65:PHE:N	1:B:66:PRO:HD3	2.25	0.52
1:S:43:PHE:HD1	1:S:59:THR:HG21	1.74	0.52
1:G:50:THR:HB	1:G:110:ARG:HH22	1.77	0.52
1:A:50:THR:HB	1:A:110:ARG:HH22	1.77	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:O	1:B:94:THR:HG23	2.10	0.52
3:K:24:ASN:HA	3:X:27:GLY:HA3	125.84	0.52
1:N:85:LEU:HD12	1:N:94:THR:O	2.10	0.52
1:B:66:PRO:HD2	3:W:19:GLU:HB3	43.32	0.52
1:A:88:ASP:CB	1:A:92:VAL:H	2.28	0.52
1:A:49:VAL:HG11	1:A:109:CYS:SG	2.51	0.52
3:Q:70:GLN:CG	1:T:71:LYS:CE	2.84	0.51
1:G:88:ASP:CB	1:G:92:VAL:H	2.22	0.51
1:B:88:ASP:CB	1:B:92:VAL:H	2.29	0.51
2:U:32:VAL:HG22	2:U:33:THR:N	2.26	0.51
2:O:102:VAL:O	2:O:103:LEU:HD12	2.10	0.51
3:L:18:TRP:CD1	3:L:25:GLN:HG3	2.46	0.51
1:N:88:ASP:CB	1:N:92:VAL:H	2.22	0.51
1:G:49:VAL:HG11	1:G:109:CYS:SG	2.50	0.51
3:L:45:TRP:CD2	3:L:95:PHE:CE1	2.97	0.51
2:D:32:VAL:HG22	2:D:33:THR:N	2.25	0.51
3:X:18:TRP:HB2	3:X:23:THR:O	2.09	0.51
2:J:72:LEU:HB3	2:J:73:HIS:CD2	2.46	0.51
3:F:40:HIS:CE1	3:F:66:CYS:HB2	2.50	0.51
1:A:49:VAL:CG1	1:A:49:VAL:O	2.59	0.51
1:M:49:VAL:O	1:M:49:VAL:CG1	2.58	0.51
1:G:49:VAL:CG1	1:G:49:VAL:O	2.58	0.51
1:M:50:THR:HB	1:M:110:ARG:HH22	1.75	0.51
1:S:92:VAL:O	1:S:94:THR:HG23	2.11	0.51
2:D:100:SER:C	2:D:101:LEU:HG	2.43	0.51
1:N:49:VAL:CG1	1:N:49:VAL:O	2.59	0.51
3:F:55:VAL:O	3:F:56:LYS:HG3	2.09	0.51
1:M:92:VAL:O	1:M:94:THR:HG23	2.11	0.51
1:M:35:TYR:O	1:N:54:HIS:NE2	2.34	0.51
3:E:40:HIS:CE1	3:E:66:CYS:HB2	2.51	0.51
2:I:38:SER:OG	2:I:39:PRO:HD2	2.13	0.51
3:F:17:ASN:ND2	3:F:20:LEU:HB3	2.26	0.51
2:C:83:GLU:O	2:C:103:LEU:HD23	2.37	0.51
3:L:47:ASN:OD1	4:L:202:NAG:O5	2.27	0.51
1:T:49:VAL:O	1:T:49:VAL:CG1	2.57	0.51
3:L:18:TRP:HB2	3:L:23:THR:O	2.12	0.50
3:E:45:TRP:CD2	3:E:95:PHE:CE1	3.03	0.50
1:N:65:PHE:N	1:N:66:PRO:HD3	2.27	0.50
3:E:96:THR:HG1	1:G:6:SER:N	2.09	0.50
1:H:43:PHE:CG	1:H:44:PRO:HA	2.46	0.50
2:V:93:HIS:HE1	2:V:94:LEU:HD12	1.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:32:VAL:HG22	2:I:33:THR:N	2.26	0.50
2:J:100:SER:OG	2:J:101:LEU:N	3.72	0.50
1:S:49:VAL:HG12	1:S:49:VAL:O	2.11	0.50
2:C:38:SER:OG	2:C:39:PRO:HD2	2.12	0.50
1:T:92:VAL:O	1:T:94:THR:HG23	2.12	0.49
1:S:11:THR:HG22	1:S:12:SER:O	2.12	0.49
2:D:59:GLU:HB2	3:W:22:ARG:NH2	34.51	0.49
2:I:53:VAL:HG12	2:I:101:LEU:CD1	2.99	0.49
1:T:49:VAL:HG11	1:T:109:CYS:SG	2.52	0.49
3:L:55:VAL:O	3:L:56:LYS:HG3	2.11	0.49
2:O:32:VAL:HG22	2:O:33:THR:N	2.27	0.49
1:G:75:VAL:HG11	1:H:75:VAL:CG1	2.45	0.49
1:B:62:HIS:HB2	1:B:69:VAL:HG12	1.94	0.49
3:Q:93:GLU:HA	3:Q:93:GLU:OE1	2.13	0.49
1:M:88:ASP:CB	1:M:92:VAL:H	2.25	0.49
2:V:38:SER:OG	2:V:39:PRO:HD2	2.12	0.49
1:N:50:THR:HB	1:N:110:ARG:HH22	1.77	0.49
1:H:64:LYS:C	1:H:66:PRO:HD3	2.32	0.49
3:R:33:GLY:HA3	3:R:39:LEU:HD21	1.94	0.49
3:L:22:ARG:NH1	3:W:10:GLU:OE2	80.33	0.49
1:G:50:THR:N	1:G:51:PRO:CD	2.85	0.49
2:D:32:VAL:HG22	2:D:33:THR:H	1.78	0.49
1:S:85:LEU:HD12	1:S:94:THR:O	2.12	0.49
1:T:88:ASP:CB	1:T:92:VAL:H	2.25	0.49
1:S:11:THR:HG22	1:S:12:SER:N	2.26	0.49
3:R:18:TRP:CD1	3:R:25:GLN:HG3	2.48	0.49
1:S:49:VAL:CG1	1:S:49:VAL:O	2.60	0.49
1:N:92:VAL:O	1:N:94:THR:HG23	2.12	0.49
1:N:11:THR:HG22	1:N:12:SER:O	2.12	0.49
3:K:18:TRP:CD1	3:K:25:GLN:HG3	2.48	0.49
2:C:32:VAL:HG22	2:C:33:THR:H	1.78	0.49
2:P:32:VAL:HG22	2:P:33:THR:H	1.78	0.49
1:S:11:THR:CG2	1:S:12:SER:N	2.76	0.49
1:G:11:THR:HG22	1:G:12:SER:O	2.19	0.49
1:G:53:LYS:HE3	2:I:75:GLU:OE2	2.13	0.49
1:T:43:PHE:CG	1:T:44:PRO:HA	2.48	0.49
2:P:100:SER:O	2:P:101:LEU:HD23	2.12	0.49
1:G:92:VAL:O	1:G:94:THR:HG23	2.13	0.49
2:J:53:VAL:HG22	2:J:67:ARG:HG2	2.03	0.49
3:K:9:ARG:HD3	3:K:10:GLU:N	2.27	0.49
1:M:15:VAL:HG21	1:N:57:VAL:HG11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:CB	2:D:84:PHE:CE1	40.29	0.48
1:B:96:LYS:HA	1:B:96:LYS:HD2	1.68	0.48
1:A:7:HIS:O	1:A:39:GLY:HA3	2.93	0.48
1:B:43:PHE:CG	1:B:44:PRO:HA	2.51	0.48
2:J:58:GLU:O	2:J:60:GLY:N	3.24	0.48
2:P:93:HIS:CE1	2:P:94:LEU:HG	2.48	0.48
2:U:72:LEU:HB3	2:U:73:HIS:CD2	2.48	0.48
4:K:201:NAG:H3	3:X:29:GLU:HG3	120.08	0.48
3:K:40:HIS:CE1	3:K:66:CYS:HB2	2.51	0.48
1:S:64:LYS:HB2	2:V:84:PHE:CZ	2.48	0.48
2:C:55:LEU:HD23	2:C:64:GLN:O	2.13	0.48
2:D:66:HIS:N	2:D:66:HIS:CD2	2.84	0.48
1:M:65:PHE:N	1:M:66:PRO:HD3	2.28	0.48
3:E:70:GLN:CG	1:G:71:LYS:CE	2.92	0.48
1:A:65:PHE:N	1:A:66:PRO:HD3	2.28	0.48
1:S:64:LYS:C	1:S:66:PRO:HD3	2.33	0.48
1:G:64:LYS:C	1:G:66:PRO:HD3	2.33	0.48
2:O:72:LEU:HA	2:O:72:LEU:HD23	1.52	0.48
3:X:18:TRP:CD1	3:X:25:GLN:HG3	2.49	0.48
1:N:43:PHE:CG	1:N:44:PRO:HA	2.49	0.48
2:P:55:LEU:HD23	2:P:64:GLN:O	2.14	0.48
1:M:96:LYS:HD2	1:M:96:LYS:HA	1.63	0.48
3:R:79:PRO:HD2	3:R:82:TYR:CZ	2.49	0.48
2:V:32:VAL:HG22	2:V:33:THR:H	1.77	0.48
1:M:20:ILE:HB	1:N:60:LEU:HD13	1.95	0.48
3:R:9:ARG:HD3	3:R:10:GLU:N	2.29	0.48
2:J:55:LEU:HB2	2:J:101:LEU:HD13	3.71	0.47
1:B:71:LYS:CE	3:W:70:GLN:CG	2.86	0.47
2:J:32:VAL:HG22	2:J:33:THR:N	2.28	0.47
1:N:10:LYS:HD3	1:N:35:TYR:CG	2.50	0.47
1:M:7:HIS:O	1:M:39:GLY:CA	2.56	0.47
1:T:96:LYS:HA	1:T:96:LYS:HD2	1.67	0.47
1:H:92:VAL:O	1:H:94:THR:HG23	2.18	0.47
1:M:93:PRO:HB2	3:Q:55:VAL:HG11	1.95	0.47
2:I:55:LEU:HD23	2:I:64:GLN:O	2.14	0.47
2:I:32:VAL:HG22	2:I:33:THR:H	1.79	0.47
2:D:72:LEU:HB3	2:D:73:HIS:CD2	2.48	0.47
2:I:66:HIS:N	2:I:66:HIS:CD2	2.82	0.47
1:H:88:ASP:CB	1:H:92:VAL:H	2.31	0.47
1:T:85:LEU:HD12	1:T:94:THR:O	2.14	0.47
1:G:60:LEU:HB3	1:H:20:ILE:HG22	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:HB2	2:D:84:PHE:CZ	40.37	0.47
1:N:50:THR:N	1:N:51:PRO:CD	2.77	0.47
1:A:79:LEU:HB3	1:A:101:GLY:HA2	2.01	0.47
1:B:49:VAL:HG11	1:B:109:CYS:SG	2.54	0.47
2:O:83:GLU:C	2:O:103:LEU:HD23	2.35	0.47
1:A:50:THR:N	1:A:51:PRO:CD	2.83	0.47
2:U:32:VAL:HG22	2:U:33:THR:H	1.80	0.47
1:G:43:PHE:CG	1:G:44:PRO:HA	2.52	0.47
1:H:11:THR:HG22	1:H:12:SER:O	2.15	0.47
1:T:50:THR:HB	1:T:110:ARG:HH22	1.78	0.47
3:X:45:TRP:CD2	3:X:95:PHE:CE1	3.03	0.47
3:K:17:ASN:ND2	3:K:20:LEU:HB3	2.30	0.47
3:E:61:LEU:O	3:E:62:ASP:C	2.53	0.47
3:E:93:GLU:OE1	3:E:93:GLU:HA	2.14	0.47
2:V:58:GLU:O	2:V:59:GLU:C	2.53	0.47
2:O:32:VAL:HG22	2:O:33:THR:H	1.80	0.47
3:X:9:ARG:HD3	3:X:10:GLU:N	2.30	0.47
1:N:77:THR:HG21	1:N:108:GLY:HA3	1.96	0.47
3:L:17:ASN:ND2	3:L:20:LEU:HB3	2.30	0.47
3:L:24:ASN:HA	3:W:27:GLY:HA3	89.01	0.47
3:E:69:ARG:HH12	2:I:61:ARG:HH11	1.57	0.47
1:A:11:THR:HG22	1:A:12:SER:N	2.29	0.47
3:E:9:ARG:HD3	3:E:10:GLU:N	2.30	0.47
1:A:64:LYS:C	1:A:66:PRO:HD3	2.37	0.46
2:O:57:ARG:O	2:O:84:PHE:HB2	2.15	0.46
1:B:50:THR:N	1:B:51:PRO:CD	2.80	0.46
2:U:53:VAL:HG22	2:U:67:ARG:HG2	1.97	0.46
1:T:79:LEU:HB3	1:T:101:GLY:HA2	1.96	0.46
3:R:17:ASN:ND2	3:R:20:LEU:HB3	2.29	0.46
1:B:7:HIS:CE1	1:B:42:PHE:HB2	9.04	0.46
2:D:72:LEU:HD23	2:D:72:LEU:HA	1.57	0.46
1:T:102:MET:HB3	1:T:102:MET:HE2	1.75	0.46
1:M:99:TYR:CE2	1:N:53:LYS:HE2	2.49	0.46
1:N:64:LYS:C	1:N:66:PRO:HD3	2.35	0.46
1:T:7:HIS:O	1:T:39:GLY:CA	2.64	0.46
1:A:77:THR:HG21	1:A:108:GLY:HA3	2.10	0.46
2:J:66:HIS:N	2:J:66:HIS:CD2	2.82	0.46
1:M:64:LYS:HB2	2:P:84:PHE:HE1	1.69	0.46
3:E:69:ARG:NH1	2:I:61:ARG:NH1	2.52	0.46
2:C:58:GLU:O	2:C:59:GLU:C	2.52	0.46
1:H:62:HIS:CD2	1:H:69:VAL:O	2.66	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:93:GLU:OE1	3:W:93:GLU:HA	2.14	0.46
3:Q:9:ARG:HD3	3:Q:10:GLU:N	2.30	0.46
1:B:11:THR:HG22	1:B:12:SER:N	2.30	0.46
1:M:64:LYS:C	1:M:66:PRO:HD3	2.36	0.46
4:K:201:NAG:H82	3:X:28:LEU:HD12	124.02	0.46
1:B:71:LYS:HE2	3:W:70:GLN:HG2	1.93	0.46
3:F:61:LEU:O	3:F:62:ASP:C	2.53	0.46
3:L:93:GLU:OE1	3:L:93:GLU:HA	2.16	0.46
3:X:40:HIS:CE1	3:X:66:CYS:HB2	2.50	0.46
3:Q:77:GLU:CG	3:Q:78:ASN:N	2.78	0.46
1:T:11:THR:HG22	1:T:12:SER:O	2.15	0.46
3:L:75:THR:O	3:L:99:PRO:HA	2.16	0.46
2:O:66:HIS:CD2	2:O:66:HIS:N	2.83	0.46
2:U:55:LEU:HD23	2:U:64:GLN:O	2.16	0.46
1:B:64:LYS:C	1:B:66:PRO:HD3	2.35	0.46
3:W:40:HIS:CE1	3:W:66:CYS:HB2	2.50	0.46
1:A:11:THR:HG22	1:A:12:SER:O	2.17	0.46
3:E:79:PRO:HD2	3:E:82:TYR:CZ	2.56	0.46
3:E:69:ARG:NH1	2:I:61:ARG:HH11	2.13	0.46
3:L:22:ARG:HD2	3:W:10:GLU:OE1	79.44	0.46
3:R:80:GLN:HG3	3:R:80:GLN:H	1.48	0.46
3:W:9:ARG:HD3	3:W:10:GLU:N	2.31	0.46
3:Q:69:ARG:NH2	2:U:61:ARG:HD2	2.30	0.46
2:C:66:HIS:CD2	2:C:66:HIS:N	2.84	0.46
3:X:75:THR:O	3:X:99:PRO:HA	2.16	0.46
1:H:77:THR:HG21	1:H:108:GLY:HA3	1.98	0.45
2:P:53:VAL:HG22	2:P:67:ARG:HG2	1.98	0.45
1:N:47:ASP:OD2	2:O:72:LEU:HG	2.17	0.45
1:B:88:ASP:HB3	1:B:92:VAL:H	1.89	0.45
3:E:79:PRO:HD2	3:E:82:TYR:CE2	2.53	0.45
4:X:202:NAG:O7	4:X:202:NAG:H3	2.15	0.45
3:E:28:LEU:C	3:E:28:LEU:HD12	2.36	0.45
2:D:53:VAL:HG22	2:D:67:ARG:HG2	1.98	0.45
1:B:85:LEU:HD12	1:B:94:THR:O	2.15	0.45
2:J:32:VAL:HG22	2:J:33:THR:H	1.81	0.45
1:M:99:TYR:HE2	1:N:53:LYS:HE2	1.82	0.45
1:B:11:THR:HG22	1:B:12:SER:O	2.19	0.45
2:V:72:LEU:HB3	2:V:73:HIS:CD2	2.51	0.45
1:S:79:LEU:HB3	1:S:101:GLY:HA2	1.98	0.45
1:S:7:HIS:CD2	1:S:7:HIS:N	2.84	0.45
3:F:79:PRO:HD2	3:F:82:TYR:CZ	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:18:TRP:CD1	3:Q:25:GLN:HG3	2.52	0.45
2:V:72:LEU:HA	2:V:72:LEU:HD23	1.54	0.45
2:V:66:HIS:N	2:V:66:HIS:CD2	2.85	0.45
2:I:102:VAL:O	2:I:103:LEU:HD23	2.16	0.45
1:G:96:LYS:HD2	1:G:96:LYS:HA	1.73	0.45
2:J:72:LEU:HD23	2:J:72:LEU:HA	1.51	0.45
1:S:88:ASP:CB	1:S:92:VAL:H	2.30	0.45
3:Q:55:VAL:O	3:Q:56:LYS:HG3	2.15	0.45
2:D:58:GLU:O	2:D:60:GLY:N	2.49	0.45
3:F:75:THR:O	3:F:99:PRO:HA	2.19	0.45
3:E:33:GLY:HA3	3:E:39:LEU:HD21	2.07	0.45
2:I:72:LEU:HB3	2:I:73:HIS:CD2	2.53	0.45
2:C:72:LEU:HD23	2:C:72:LEU:HA	1.50	0.45
1:G:62:HIS:HB2	1:G:69:VAL:HG12	1.98	0.45
1:H:96:LYS:HD2	1:H:96:LYS:HA	1.70	0.45
3:E:75:THR:O	3:E:99:PRO:HA	2.21	0.45
3:E:98:LEU:HA	3:E:99:PRO:HD2	1.89	0.45
2:U:38:SER:OG	2:U:39:PRO:HD2	2.16	0.45
1:B:10:LYS:HD3	1:B:35:TYR:CG	2.51	0.45
1:S:75:VAL:HG11	1:T:75:VAL:CG1	2.43	0.45
2:J:58:GLU:O	2:J:59:GLU:C	2.56	0.45
1:H:50:THR:N	1:H:51:PRO:CD	2.80	0.45
2:O:72:LEU:HB3	2:O:73:HIS:CD2	2.52	0.45
2:C:72:LEU:HB3	2:C:73:HIS:CD2	2.54	0.45
1:H:95:LEU:HD22	3:L:42:TYR:OH	2.18	0.45
1:M:43:PHE:CG	1:M:44:PRO:HA	2.52	0.45
1:N:66:PRO:HG2	2:O:59:GLU:HB3	1.99	0.45
1:T:65:PHE:N	1:T:66:PRO:HD3	2.31	0.45
1:M:50:THR:N	1:M:51:PRO:CD	2.80	0.45
3:F:33:GLY:HA3	3:F:39:LEU:HD21	1.98	0.45
1:B:62:HIS:CD2	1:B:69:VAL:O	2.65	0.45
1:A:25:TRP:CH2	1:A:26:ILE:HD11	2.61	0.45
3:F:9:ARG:HD3	3:F:10:GLU:N	2.31	0.45
1:N:25:TRP:CH2	1:N:26:ILE:HD11	2.52	0.45
1:B:79:LEU:HB3	1:B:101:GLY:HA2	1.98	0.45
1:A:95:LEU:HD22	3:E:42:TYR:CZ	2.52	0.45
1:H:7:HIS:HB3	1:H:8:CYS:H	1.62	0.44
1:G:79:LEU:HB3	1:G:101:GLY:HA2	1.99	0.44
1:A:7:HIS:O	1:A:9:GLN:HG2	2.17	0.44
3:X:82:TYR:OH	4:X:202:NAG:H83	2.17	0.44
3:Q:75:THR:O	3:Q:99:PRO:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:80:GLN:H	3:K:80:GLN:HG3	1.46	0.44
2:I:55:LEU:O	2:I:85:VAL:HA	2.17	0.44
1:S:75:VAL:CG1	1:T:75:VAL:HG11	2.43	0.44
2:C:83:GLU:C	2:C:103:LEU:HD23	3.00	0.44
3:Q:40:HIS:CE1	3:Q:66:CYS:HB2	2.52	0.44
3:K:47:ASN:OD1	4:K:202:NAG:O5	2.71	0.44
1:H:88:ASP:HB3	1:H:92:VAL:H	1.89	0.44
1:M:88:ASP:HB3	1:M:92:VAL:H	1.82	0.44
1:G:11:THR:HG22	1:G:12:SER:N	2.36	0.44
1:M:20:ILE:CG2	1:N:60:LEU:HB3	2.47	0.44
1:M:20:ILE:HG22	1:N:60:LEU:HB3	1.98	0.44
3:L:79:PRO:HD2	3:L:82:TYR:CE2	2.55	0.44
3:F:18:TRP:CD1	3:F:25:GLN:HG3	2.58	0.44
1:A:43:PHE:CG	1:A:44:PRO:HA	2.53	0.44
3:L:28:LEU:HD12	3:L:28:LEU:C	2.38	0.44
1:G:88:ASP:HB3	1:G:92:VAL:H	1.83	0.44
1:H:23:ASP:OD2	2:I:80:ARG:NH1	2.75	0.44
3:L:64:PHE:HA	3:L:67:TYR:CD2	2.58	0.44
1:M:94:THR:HA	3:Q:56:LYS:HE2	1.99	0.44
1:G:60:LEU:HD13	1:H:20:ILE:HB	2.24	0.44
1:B:11:THR:CG2	1:B:12:SER:N	2.80	0.44
3:W:61:LEU:O	3:W:62:ASP:C	2.55	0.44
3:L:61:LEU:O	3:L:62:ASP:C	2.58	0.44
3:L:38:ARG:HD3	3:L:87:GLU:OE2	2.18	0.44
2:U:66:HIS:CD2	2:U:66:HIS:N	2.83	0.44
1:G:10:LYS:HD3	1:G:35:TYR:CG	2.52	0.44
1:T:62:HIS:HB2	1:T:69:VAL:HG12	1.98	0.44
3:Q:18:TRP:CE2	3:Q:19:GLU:HG2	2.52	0.44
3:K:79:PRO:HD2	3:K:82:TYR:CE2	2.60	0.44
3:K:38:ARG:HD3	3:K:87:GLU:OE2	2.21	0.44
2:P:66:HIS:N	2:P:66:HIS:CD2	2.84	0.44
4:Q:202:NAG:H3	4:Q:202:NAG:H82	1.98	0.44
2:C:55:LEU:O	2:C:85:VAL:HA	2.18	0.43
1:T:88:ASP:HB3	1:T:92:VAL:H	1.83	0.43
1:T:50:THR:N	1:T:51:PRO:CD	2.80	0.43
1:A:97:TYR:CE1	3:E:61:LEU:HG	2.86	0.43
3:L:17:ASN:HD21	3:L:20:LEU:HD23	1.83	0.43
1:G:77:THR:HG21	1:G:108:GLY:HA3	2.02	0.43
3:Q:28:LEU:C	3:Q:28:LEU:HD12	2.39	0.43
3:W:80:GLN:HG3	3:W:80:GLN:H	1.45	0.43
3:R:93:GLU:HA	3:R:93:GLU:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:59:GLU:C	2:V:61:ARG:H	2.16	0.43
1:N:24:SER:OG	1:N:25:TRP:HD1	2.01	0.43
3:Q:61:LEU:O	3:Q:62:ASP:C	2.55	0.43
2:D:92:SER:OG	2:D:95:CYS:HB3	2.18	0.43
1:A:11:THR:CG2	1:A:12:SER:N	2.81	0.43
1:B:95:LEU:HD22	3:F:42:TYR:CZ	2.80	0.43
2:J:55:LEU:HD23	2:J:64:GLN:O	2.18	0.43
1:B:65:PHE:HD2	3:W:19:GLU:OE1	48.48	0.43
2:D:100:SER:OG	2:D:101:LEU:N	2.63	0.43
1:T:47:ASP:C	1:T:49:VAL:H	2.21	0.43
1:N:47:ASP:C	1:N:49:VAL:H	2.22	0.43
1:T:63:LEU:HA	1:T:63:LEU:HD23	1.88	0.43
1:G:7:HIS:CG	2:I:40:HIS:HE2	4.28	0.43
1:B:94:THR:HG22	3:F:21:GLU:OE2	2.19	0.43
2:P:55:LEU:O	2:P:85:VAL:HA	2.18	0.43
3:L:9:ARG:HD3	3:L:10:GLU:N	2.34	0.43
3:Q:79:PRO:HD2	3:Q:82:TYR:CE2	2.52	0.43
1:B:32:TYR:CZ	1:B:34:ALA:HB2	2.64	0.43
3:F:80:GLN:H	3:F:80:GLN:HG3	1.50	0.43
2:V:53:VAL:HG22	2:V:67:ARG:HG2	1.99	0.43
1:T:62:HIS:CD2	1:T:69:VAL:O	2.68	0.43
3:F:61:LEU:O	3:F:63:ASP:N	2.58	0.43
2:V:55:LEU:O	2:V:85:VAL:HA	2.19	0.43
2:D:55:LEU:HD23	2:D:64:GLN:O	2.18	0.43
1:B:71:LYS:HD2	3:W:70:GLN:CG	2.47	0.43
1:B:32:TYR:CE2	1:B:34:ALA:HB2	2.64	0.43
2:P:72:LEU:HB3	2:P:73:HIS:CD2	2.54	0.43
1:H:25:TRP:CH2	1:H:26:ILE:HD11	2.54	0.43
3:X:79:PRO:HD2	3:X:82:TYR:CE2	2.53	0.43
3:K:33:GLY:HA3	3:K:39:LEU:HD21	1.99	0.43
1:S:50:THR:N	1:S:51:PRO:CD	2.82	0.43
2:D:53:VAL:HG12	2:D:101:LEU:HD11	2.00	0.43
1:G:23:ASP:OD1	1:G:23:ASP:N	2.59	0.43
3:W:28:LEU:HD12	3:W:28:LEU:C	2.39	0.43
1:A:23:ASP:OD1	1:A:23:ASP:N	2.60	0.43
2:O:55:LEU:O	2:O:85:VAL:HA	2.18	0.42
3:Q:94:ARG:CD	1:T:38:LYS:HE2	2.49	0.42
1:T:64:LYS:C	1:T:66:PRO:HD3	2.40	0.42
1:H:43:PHE:HD1	1:H:59:THR:HG21	1.87	0.42
3:K:61:LEU:O	3:K:62:ASP:C	2.56	0.42
3:R:28:LEU:C	3:R:28:LEU:HD12	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:28:LEU:C	3:X:28:LEU:HD12	2.40	0.42
3:L:18:TRP:CE2	3:L:19:GLU:HG2	2.54	0.42
1:M:47:ASP:C	1:M:49:VAL:H	2.22	0.42
1:G:60:LEU:HB3	1:H:20:ILE:CG2	2.70	0.42
2:O:53:VAL:HG22	2:O:67:ARG:HG2	2.01	0.42
3:R:75:THR:O	3:R:99:PRO:HA	2.18	0.42
3:L:80:GLN:HG3	3:L:80:GLN:H	1.44	0.42
1:T:10:LYS:HD3	1:T:35:TYR:CG	2.54	0.42
1:N:96:LYS:HD2	1:N:96:LYS:HA	1.71	0.42
1:H:62:HIS:HB2	1:H:69:VAL:HG12	2.01	0.42
1:S:43:PHE:CG	1:S:44:PRO:HA	2.54	0.42
1:G:11:THR:CG2	1:G:12:SER:N	2.86	0.42
3:F:98:LEU:HA	3:F:99:PRO:HD2	1.93	0.42
3:E:93:GLU:HG2	1:H:67:THR:O	2.19	0.42
3:E:70:GLN:CG	1:G:71:LYS:HE3	2.42	0.42
2:V:53:VAL:HG23	2:V:96:ASN:HB2	2.00	0.42
2:J:94:LEU:HA	2:J:94:LEU:HD23	1.69	0.42
3:F:28:LEU:C	3:F:28:LEU:HD12	2.39	0.42
1:A:62:HIS:HB2	1:A:69:VAL:HG12	2.01	0.42
1:N:79:LEU:HB3	1:N:101:GLY:HA2	2.02	0.42
2:I:53:VAL:HG22	2:I:67:ARG:HG2	2.02	0.42
3:R:44:SER:HA	3:R:82:TYR:O	2.20	0.42
1:G:47:ASP:C	1:G:49:VAL:H	2.28	0.42
1:T:43:PHE:HD1	1:T:59:THR:HG21	1.84	0.42
1:H:11:THR:CG2	1:H:12:SER:N	2.83	0.42
2:P:72:LEU:HA	2:P:72:LEU:HD23	1.60	0.42
1:G:62:HIS:CD2	1:G:69:VAL:O	2.69	0.42
3:F:17:ASN:HD21	3:F:20:LEU:HD23	1.86	0.42
1:H:11:THR:HG22	1:H:12:SER:N	2.34	0.42
1:S:25:TRP:CH2	1:S:26:ILE:HD11	2.54	0.42
2:P:59:GLU:H	2:P:59:GLU:HG2	1.54	0.42
2:D:55:LEU:O	2:D:85:VAL:HA	2.20	0.42
2:C:53:VAL:HG23	2:C:96:ASN:HB2	2.02	0.42
1:A:88:ASP:HB3	1:A:92:VAL:H	1.85	0.42
1:S:62:HIS:HB2	1:S:69:VAL:HG12	2.01	0.42
3:X:47:ASN:OD1	4:X:202:NAG:O5	2.30	0.42
1:H:23:ASP:CG	2:I:80:ARG:HH11	2.34	0.42
3:R:82:TYR:N	3:R:82:TYR:CD2	2.88	0.42
3:R:61:LEU:O	3:R:62:ASP:C	2.58	0.42
4:L:201:NAG:H3	3:W:29:GLU:HG3	89.90	0.42
1:H:32:TYR:CZ	1:H:34:ALA:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:LEU:HB3	1:H:101:GLY:HA2	2.02	0.42
3:E:22:ARG:HD3	3:E:22:ARG:HA	1.89	0.42
1:T:23:ASP:N	1:T:23:ASP:OD1	2.52	0.42
1:T:53:LYS:HE3	2:U:75:GLU:OE2	2.20	0.42
1:A:10:LYS:HD3	1:A:35:TYR:CG	2.57	0.42
1:N:63:LEU:HA	1:N:63:LEU:HD23	1.90	0.42
2:P:100:SER:C	2:P:101:LEU:HG	2.40	0.42
3:K:20:LEU:HA	3:K:20:LEU:HD12	1.90	0.42
3:X:61:LEU:O	3:X:62:ASP:C	2.59	0.42
1:M:79:LEU:HB3	1:M:101:GLY:HA2	2.01	0.42
3:K:22:ARG:HA	3:X:28:LEU:HD21	131.30	0.41
3:K:75:THR:O	3:K:99:PRO:HA	2.19	0.41
3:X:22:ARG:HA	3:X:22:ARG:HD3	1.87	0.41
2:P:76:LEU:HD23	2:P:76:LEU:HA	1.93	0.41
2:J:55:LEU:O	2:J:85:VAL:HA	2.20	0.41
1:S:96:LYS:HD2	1:S:96:LYS:HA	1.68	0.41
2:C:53:VAL:HG22	2:C:67:ARG:HG2	2.02	0.41
1:M:15:VAL:HG21	1:N:57:VAL:CG1	2.49	0.41
3:E:38:ARG:HD3	3:E:87:GLU:OE2	2.25	0.41
3:Q:20:LEU:HA	3:Q:20:LEU:HD23	1.95	0.41
2:J:56:VAL:O	2:J:63:PRO:HA	2.29	0.41
3:K:13:TYR:CZ	4:X:201:NAG:H62	120.04	0.41
2:I:53:VAL:HG23	2:I:96:ASN:HB2	2.03	0.41
1:A:96:LYS:HA	1:A:96:LYS:HD2	1.65	0.41
1:N:62:HIS:CD2	1:N:69:VAL:O	2.70	0.41
1:B:47:ASP:C	1:B:49:VAL:H	2.26	0.41
1:N:49:VAL:CG1	1:N:109:CYS:HB2	2.51	0.41
2:I:72:LEU:HD23	2:I:72:LEU:HA	1.45	0.41
3:L:79:PRO:HG2	3:L:82:TYR:CD2	2.72	0.41
1:A:66:PRO:HG2	2:C:59:GLU:CB	28.56	0.41
3:R:20:LEU:HD12	3:R:20:LEU:HA	1.89	0.41
1:N:23:ASP:N	1:N:23:ASP:OD1	2.54	0.41
1:S:63:LEU:HD23	1:S:63:LEU:HA	1.91	0.41
3:R:12:ILE:HB	3:R:92:ASN:OD1	2.19	0.41
1:H:10:LYS:HD3	1:H:35:TYR:CG	2.56	0.41
2:C:57:ARG:O	2:C:59:GLU:N	3.52	0.41
2:C:58:GLU:C	2:C:60:GLY:H	4.25	0.41
1:A:49:VAL:CG1	1:A:109:CYS:HB2	2.54	0.41
3:E:64:PHE:HA	3:E:67:TYR:CD2	2.58	0.41
2:C:55:LEU:HD13	2:C:103:LEU:HD11	2.58	0.41
2:J:53:VAL:HG23	2:J:96:ASN:HB2	2.05	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:83:GLU:O	2:O:103:LEU:HD23	2.21	0.41
1:N:64:LYS:HD2	2:O:84:PHE:HE1	1.86	0.41
1:G:66:PRO:HG3	2:I:59:GLU:HB3	4.66	0.41
3:Q:18:TRP:CG	3:Q:19:GLU:N	2.88	0.41
3:W:75:THR:O	3:W:99:PRO:HA	2.20	0.41
3:F:51:THR:CG2	3:F:51:THR:O	2.68	0.41
2:O:60:GLY:O	2:O:61:ARG:O	2.38	0.41
2:D:56:VAL:O	2:D:63:PRO:HA	2.32	0.41
1:A:71:LYS:NZ	2:D:59:GLU:OE2	2.54	0.41
1:H:53:LYS:HD2	2:J:73:HIS:CE1	2.56	0.41
3:F:18:TRP:CE2	3:F:19:GLU:HG2	2.57	0.41
3:X:18:TRP:CE2	3:X:19:GLU:HG2	2.55	0.41
1:N:52:THR:HG23	1:N:110:ARG:HD3	2.03	0.41
2:O:53:VAL:HG23	2:O:96:ASN:HB2	2.02	0.41
3:E:80:GLN:HG3	3:E:80:GLN:H	1.45	0.41
1:A:62:HIS:CD2	1:A:69:VAL:O	2.73	0.41
3:W:18:TRP:CD1	3:W:25:GLN:HG3	2.56	0.41
3:X:79:PRO:HD2	3:X:82:TYR:CZ	2.56	0.41
3:F:12:ILE:HA	3:F:12:ILE:HD13	1.88	0.41
1:A:52:THR:HG23	1:A:110:ARG:HD3	2.11	0.40
1:N:88:ASP:HB2	1:N:92:VAL:H	1.85	0.40
3:K:61:LEU:HD23	3:K:61:LEU:HA	1.84	0.40
1:G:24:SER:OG	1:G:25:TRP:HD1	2.04	0.40
3:W:38:ARG:HD3	3:W:87:GLU:OE2	2.21	0.40
1:A:60:LEU:O	1:A:63:LEU:HB2	2.21	0.40
2:O:56:VAL:O	2:O:63:PRO:HA	2.21	0.40
1:G:102:MET:HE2	1:G:102:MET:HB3	1.91	0.40
3:E:12:ILE:HD13	3:E:12:ILE:HA	1.91	0.40
1:A:64:LYS:HD2	2:C:84:PHE:HE1	43.08	0.40
3:Q:79:PRO:HD2	3:Q:82:TYR:CZ	2.57	0.40
2:U:55:LEU:O	2:U:85:VAL:HA	2.21	0.40
2:C:57:ARG:C	2:C:59:GLU:H	4.26	0.40
1:A:47:ASP:C	1:A:49:VAL:H	2.26	0.40
3:K:18:TRP:CE2	3:K:19:GLU:HG2	2.56	0.40
1:S:94:THR:HG22	3:W:21:GLU:OE2	2.21	0.40
2:V:55:LEU:HD23	2:V:64:GLN:O	2.21	0.40
1:M:11:THR:HG22	1:M:12:SER:N	2.36	0.40
1:G:32:TYR:CZ	1:G:34:ALA:HB2	2.56	0.40
1:G:7:HIS:ND1	2:I:40:HIS:NE2	5.17	0.40
1:A:95:LEU:HD22	3:E:42:TYR:OH	2.21	0.40
1:B:95:LEU:HD22	3:F:42:TYR:OH	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:93:HIS:CE1	2:J:94:LEU:HG	2.98	0.40
1:G:25:TRP:CH2	1:G:26:ILE:HD11	2.58	0.40
2:D:57:ARG:HG2	3:W:20:LEU:HD21	38.77	0.40
1:N:96:LYS:HE3	1:N:98:HIS:N	2.34	0.40
1:B:109:CYS:C	1:B:110:ARG:HG2	2.45	0.40
3:F:44:SER:HA	3:F:82:TYR:O	2.22	0.40
1:M:94:THR:HG22	3:Q:21:GLU:OE2	2.22	0.40
3:Q:82:TYR:CD2	3:Q:82:TYR:N	2.89	0.40
1:B:77:THR:HG21	1:B:108:GLY:HA3	2.03	0.40
1:G:61:VAL:HG21	1:H:15:VAL:HG22	2.10	0.40
2:U:56:VAL:O	2:U:63:PRO:HA	2.21	0.40
2:I:78:ARG:H	2:I:78:ARG:HG2	1.69	0.40

There are no symmetry-related clashes.

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	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	19	60
1	B	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	19	60
1	G	103/110 (94%)	94 (91%)	9 (9%)	0	100	100
1	H	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	10	46
1	M	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	10	46
1	N	102/110 (93%)	93 (91%)	8 (8%)	1 (1%)	19	60
1	S	103/110 (94%)	94 (91%)	8 (8%)	1 (1%)	19	60
1	T	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	19	60
1	a	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	10	46
1	b	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	19	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	19	60
1	h	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	19	60
2	C	73/106 (69%)	57 (78%)	12 (16%)	4 (6%)	2	18
2	D	70/106 (66%)	55 (79%)	11 (16%)	4 (6%)	2	17
2	I	73/106 (69%)	54 (74%)	15 (20%)	4 (6%)	2	18
2	J	70/106 (66%)	54 (77%)	12 (17%)	4 (6%)	2	17
2	O	73/106 (69%)	57 (78%)	12 (16%)	4 (6%)	2	18
2	P	70/106 (66%)	56 (80%)	10 (14%)	4 (6%)	2	17
2	U	73/106 (69%)	57 (78%)	13 (18%)	3 (4%)	3	27
2	V	70/106 (66%)	56 (80%)	10 (14%)	4 (6%)	2	17
2	c	73/106 (69%)	54 (74%)	15 (20%)	4 (6%)	2	18
2	d	70/106 (66%)	56 (80%)	11 (16%)	3 (4%)	3	26
2	i	73/106 (69%)	56 (77%)	13 (18%)	4 (6%)	2	18
2	j	70/106 (66%)	55 (79%)	11 (16%)	4 (6%)	2	17
3	E	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	17	58
3	F	89/124 (72%)	77 (86%)	10 (11%)	2 (2%)	8	43
3	K	89/124 (72%)	76 (85%)	11 (12%)	2 (2%)	8	43
3	L	89/124 (72%)	79 (89%)	9 (10%)	1 (1%)	17	58
3	Q	89/124 (72%)	79 (89%)	9 (10%)	1 (1%)	17	58
3	R	89/124 (72%)	77 (86%)	11 (12%)	1 (1%)	17	58
3	W	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	17	58
3	X	89/124 (72%)	77 (86%)	11 (12%)	1 (1%)	17	58
3	e	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	17	58
3	f	89/124 (72%)	79 (89%)	8 (9%)	2 (2%)	8	43
3	k	89/124 (72%)	76 (85%)	11 (12%)	2 (2%)	8	43
3	l	89/124 (72%)	79 (89%)	8 (9%)	2 (2%)	8	43
All	All	3161/4080 (78%)	2736 (87%)	348 (11%)	77 (2%)	7	41

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	62	ASP
3	F	62	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	88	ASP
3	K	62	ASP
3	L	62	ASP
1	M	88	ASP
2	O	61	ARG
2	P	59	GLU
3	Q	62	ASP
3	R	62	ASP
3	W	62	ASP
3	X	62	ASP
3	e	62	ASP
3	f	62	ASP
2	i	58	GLU
2	j	59	GLU
3	k	62	ASP
3	l	62	ASP
1	A	88	ASP
1	B	88	ASP
2	C	59	GLU
2	D	61	ARG
2	J	59	GLU
1	S	88	ASP
1	T	88	ASP
2	V	59	GLU
1	a	7	HIS
1	a	88	ASP
1	b	88	ASP
2	c	58	GLU
1	h	88	ASP
2	C	94	LEU
2	C	98	ASN
2	D	94	LEU
2	I	94	LEU
2	I	98	ASN
2	J	94	LEU
2	J	98	ASN
1	N	88	ASP
2	P	94	LEU
2	U	98	ASN
2	c	94	LEU
2	c	98	ASN
2	i	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	i	98	ASN
2	j	94	LEU
2	D	98	ASN
1	H	7	HIS
2	I	61	ARG
3	K	17	ASN
2	O	98	ASN
2	P	98	ASN
2	V	98	ASN
2	d	94	LEU
2	d	98	ASN
3	f	35	GLN
1	g	88	ASP
2	j	98	ASN
2	C	99	VAL
2	D	99	VAL
3	F	17	ASN
2	I	99	VAL
2	J	99	VAL
2	O	94	LEU
2	O	99	VAL
2	U	94	LEU
2	V	94	LEU
2	V	99	VAL
2	c	99	VAL
2	d	99	VAL
2	i	99	VAL
1	M	7	HIS
2	P	99	VAL
2	U	99	VAL
2	j	99	VAL
3	k	17	ASN
3	l	35	GLN

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	91/93 (98%)	88 (97%)	3 (3%)	45	79
1	B	89/93 (96%)	85 (96%)	4 (4%)	34	72
1	G	88/93 (95%)	85 (97%)	3 (3%)	44	78
1	H	91/93 (98%)	88 (97%)	3 (3%)	45	79
1	M	90/93 (97%)	87 (97%)	3 (3%)	45	79
1	N	87/93 (94%)	84 (97%)	3 (3%)	44	78
1	S	91/93 (98%)	88 (97%)	3 (3%)	45	79
1	T	89/93 (96%)	85 (96%)	4 (4%)	34	72
1	a	87/93 (94%)	84 (97%)	3 (3%)	44	78
1	b	91/93 (98%)	88 (97%)	3 (3%)	45	79
1	g	91/93 (98%)	88 (97%)	3 (3%)	45	79
1	h	91/93 (98%)	88 (97%)	3 (3%)	45	79
2	C	63/92 (68%)	56 (89%)	7 (11%)	8	30
2	D	63/92 (68%)	54 (86%)	9 (14%)	4	19
2	I	58/92 (63%)	49 (84%)	9 (16%)	3	16
2	J	59/92 (64%)	51 (86%)	8 (14%)	5	21
2	O	55/92 (60%)	48 (87%)	7 (13%)	5	24
2	P	60/92 (65%)	53 (88%)	7 (12%)	7	28
2	U	64/92 (70%)	55 (86%)	9 (14%)	4	19
2	V	62/92 (67%)	53 (86%)	9 (14%)	4	18
2	c	61/92 (66%)	54 (88%)	7 (12%)	7	28
2	d	59/92 (64%)	51 (86%)	8 (14%)	5	21
2	i	62/92 (67%)	54 (87%)	8 (13%)	5	23
2	j	64/92 (70%)	55 (86%)	9 (14%)	4	19
3	E	76/106 (72%)	70 (92%)	6 (8%)	15	50
3	F	73/106 (69%)	68 (93%)	5 (7%)	20	58
3	K	71/106 (67%)	66 (93%)	5 (7%)	19	57
3	L	75/106 (71%)	69 (92%)	6 (8%)	15	50
3	Q	77/106 (73%)	67 (87%)	10 (13%)	5	22
3	R	73/106 (69%)	66 (90%)	7 (10%)	10	38
3	W	75/106 (71%)	66 (88%)	9 (12%)	6	26
3	X	72/106 (68%)	64 (89%)	8 (11%)	8	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	e	73/106 (69%)	68 (93%)	5 (7%)	20	58
3	f	76/106 (72%)	70 (92%)	6 (8%)	15	50
3	k	72/106 (68%)	66 (92%)	6 (8%)	14	48
3	l	72/106 (68%)	65 (90%)	7 (10%)	10	38
All	All	2691/3492 (77%)	2476 (92%)	215 (8%)	15	50

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	96	LYS
1	A	98	HIS
1	B	7	HIS
1	B	50	THR
1	B	96	LYS
1	B	98	HIS
2	C	54	VAL
2	C	55	LEU
2	C	71	ASN
2	C	80	ARG
2	C	87	HIS
2	C	91	ASP
2	C	99	VAL
2	D	54	VAL
2	D	55	LEU
2	D	57	ARG
2	D	71	ASN
2	D	80	ARG
2	D	87	HIS
2	D	91	ASP
2	D	99	VAL
2	D	101	LEU
3	E	20	LEU
3	E	23	THR
3	E	54	LEU
3	E	80	GLN
3	E	94	ARG
3	E	98	LEU
3	F	23	THR
3	F	51	THR
3	F	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	80	GLN
3	F	98	LEU
1	G	50	THR
1	G	96	LYS
1	G	98	HIS
1	H	50	THR
1	H	96	LYS
1	H	98	HIS
2	I	54	VAL
2	I	55	LEU
2	I	58	GLU
2	I	71	ASN
2	I	80	ARG
2	I	87	HIS
2	I	91	ASP
2	I	99	VAL
2	I	103	LEU
2	J	54	VAL
2	J	55	LEU
2	J	71	ASN
2	J	80	ARG
2	J	87	HIS
2	J	91	ASP
2	J	99	VAL
2	J	100	SER
3	K	23	THR
3	K	54	LEU
3	K	80	GLN
3	K	82	TYR
3	K	98	LEU
3	L	23	THR
3	L	26	SER
3	L	54	LEU
3	L	80	GLN
3	L	82	TYR
3	L	98	LEU
1	M	50	THR
1	M	96	LYS
1	M	98	HIS
1	N	50	THR
1	N	96	LYS
1	N	98	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	54	VAL
2	O	55	LEU
2	O	71	ASN
2	O	80	ARG
2	O	87	HIS
2	O	91	ASP
2	O	99	VAL
2	P	54	VAL
2	P	55	LEU
2	P	71	ASN
2	P	80	ARG
2	P	87	HIS
2	P	91	ASP
2	P	99	VAL
3	Q	20	LEU
3	Q	23	THR
3	Q	26	SER
3	Q	54	LEU
3	Q	77	GLU
3	Q	80	GLN
3	Q	82	TYR
3	Q	84	CYS
3	Q	94	ARG
3	Q	98	LEU
3	R	23	THR
3	R	26	SER
3	R	36	ASP
3	R	54	LEU
3	R	80	GLN
3	R	82	TYR
3	R	98	LEU
1	S	50	THR
1	S	96	LYS
1	S	98	HIS
1	T	7	HIS
1	T	50	THR
1	T	96	LYS
1	T	98	HIS
2	U	54	VAL
2	U	55	LEU
2	U	71	ASN
2	U	80	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	U	87	HIS
2	U	91	ASP
2	U	99	VAL
2	U	100	SER
2	U	102	VAL
2	V	54	VAL
2	V	55	LEU
2	V	58	GLU
2	V	59	GLU
2	V	71	ASN
2	V	80	ARG
2	V	87	HIS
2	V	91	ASP
2	V	99	VAL
3	W	20	LEU
3	W	23	THR
3	W	51	THR
3	W	54	LEU
3	W	80	GLN
3	W	82	TYR
3	W	84	CYS
3	W	94	ARG
3	W	98	LEU
3	X	23	THR
3	X	26	SER
3	X	48	SER
3	X	51	THR
3	X	54	LEU
3	X	80	GLN
3	X	82	TYR
3	X	98	LEU
1	a	50	THR
1	a	96	LYS
1	a	98	HIS
1	b	50	THR
1	b	96	LYS
1	b	98	HIS
2	c	54	VAL
2	c	55	LEU
2	c	71	ASN
2	c	80	ARG
2	c	87	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	c	91	ASP
2	c	99	VAL
2	d	54	VAL
2	d	55	LEU
2	d	71	ASN
2	d	80	ARG
2	d	87	HIS
2	d	91	ASP
2	d	94	LEU
2	d	101	LEU
3	e	23	THR
3	e	54	LEU
3	e	80	GLN
3	e	82	TYR
3	e	98	LEU
3	f	23	THR
3	f	54	LEU
3	f	80	GLN
3	f	82	TYR
3	f	84	CYS
3	f	98	LEU
1	g	50	THR
1	g	96	LYS
1	g	98	HIS
1	h	50	THR
1	h	96	LYS
1	h	98	HIS
2	i	54	VAL
2	i	55	LEU
2	i	59	GLU
2	i	71	ASN
2	i	80	ARG
2	i	87	HIS
2	i	91	ASP
2	i	99	VAL
2	j	54	VAL
2	j	55	LEU
2	j	57	ARG
2	j	71	ASN
2	j	80	ARG
2	j	87	HIS
2	j	91	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	j	99	VAL
2	j	101	LEU
3	k	23	THR
3	k	51	THR
3	k	54	LEU
3	k	80	GLN
3	k	82	TYR
3	k	98	LEU
3	l	23	THR
3	l	26	SER
3	l	54	LEU
3	l	80	GLN
3	l	82	TYR
3	l	84	CYS
3	l	98	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	B	62	HIS
2	C	66	HIS
3	E	17	ASN
3	F	17	ASN
1	G	62	HIS
1	H	62	HIS
3	K	17	ASN
3	L	17	ASN
1	M	62	HIS
1	N	62	HIS
2	P	93	HIS
3	R	17	ASN
1	S	62	HIS
1	T	62	HIS
2	U	66	HIS
2	V	66	HIS
2	V	93	HIS
3	X	17	ASN
1	a	62	HIS
1	b	7	HIS
1	b	62	HIS
2	d	93	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	e	17	ASN
3	f	17	ASN
1	g	62	HIS
1	h	54	HIS
1	h	62	HIS
3	k	17	ASN
3	l	17	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	201	3	14,14,15	0.65	0	15,19,21	1.48	3 (20%)
4	NAG	E	202	3	14,14,15	0.65	0	15,19,21	2.33	4 (26%)
4	NAG	F	201	3	14,14,15	0.46	0	15,19,21	1.60	3 (20%)
4	NAG	F	202	3	14,14,15	0.58	0	15,19,21	1.16	1 (6%)
4	NAG	K	201	3	14,14,15	0.48	0	15,19,21	1.98	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	202	3	14,14,15	0.77	1 (7%)	15,19,21	2.14	4 (26%)
4	NAG	L	201	3	14,14,15	0.74	0	15,19,21	1.53	1 (6%)
4	NAG	L	202	3	14,14,15	0.75	0	15,19,21	1.49	3 (20%)
4	NAG	Q	201	3	14,14,15	0.65	0	15,19,21	1.27	3 (20%)
4	NAG	Q	202	3	14,14,15	0.79	1 (7%)	15,19,21	2.22	5 (33%)
4	NAG	R	201	3	14,14,15	0.74	0	15,19,21	1.30	2 (13%)
4	NAG	R	202	3	14,14,15	0.57	0	15,19,21	1.32	2 (13%)
4	NAG	W	201	3	14,14,15	0.61	0	15,19,21	2.24	2 (13%)
4	NAG	W	202	3	14,14,15	0.54	0	15,19,21	1.92	4 (26%)
4	NAG	X	201	3	14,14,15	0.54	0	15,19,21	1.22	1 (6%)
4	NAG	X	202	3	14,14,15	0.76	0	15,19,21	1.58	5 (33%)
4	NAG	e	201	3	14,14,15	0.57	0	15,19,21	1.61	3 (20%)
4	NAG	e	202	3	14,14,15	0.59	0	15,19,21	1.23	1 (6%)
4	NAG	f	201	3	14,14,15	0.66	0	15,19,21	1.38	2 (13%)
4	NAG	f	202	3	14,14,15	0.51	0	15,19,21	1.85	3 (20%)
4	NAG	k	201	3	14,14,15	0.51	0	15,19,21	2.19	4 (26%)
4	NAG	k	202	3	14,14,15	0.49	0	15,19,21	0.77	0
4	NAG	l	201	3	14,14,15	0.69	0	15,19,21	1.52	4 (26%)
4	NAG	l	202	3	14,14,15	0.57	0	15,19,21	1.39	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	201	3	-	0/6/23/26	0/1/1/1
4	NAG	E	202	3	-	1/6/23/26	0/1/1/1
4	NAG	F	201	3	-	0/6/23/26	0/1/1/1
4	NAG	F	202	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	K	201	3	-	0/6/23/26	0/1/1/1
4	NAG	K	202	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	L	201	3	-	0/6/23/26	0/1/1/1
4	NAG	L	202	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	Q	201	3	-	0/6/23/26	0/1/1/1
4	NAG	Q	202	3	-	1/6/23/26	0/1/1/1
4	NAG	R	201	3	-	0/6/23/26	0/1/1/1
4	NAG	R	202	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	W	201	3	-	0/6/23/26	0/1/1/1
4	NAG	W	202	3	-	0/6/23/26	0/1/1/1
4	NAG	X	201	3	-	1/6/23/26	0/1/1/1
4	NAG	X	202	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	e	201	3	-	0/6/23/26	0/1/1/1
4	NAG	e	202	3	-	0/6/23/26	0/1/1/1
4	NAG	f	201	3	-	0/6/23/26	0/1/1/1
4	NAG	f	202	3	-	0/6/23/26	0/1/1/1
4	NAG	k	201	3	-	0/6/23/26	0/1/1/1
4	NAG	k	202	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	l	201	3	-	0/6/23/26	0/1/1/1
4	NAG	l	202	3	1/1/5/7	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	202	NAG	C1-C2	2.28	1.55	1.52
4	Q	202	NAG	C1-C2	2.35	1.55	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	201	NAG	C2-N2-C7	-7.04	114.00	123.04
4	L	201	NAG	C2-N2-C7	-4.39	117.40	123.04
4	f	202	NAG	C4-C3-C2	-4.26	104.60	111.23
4	k	201	NAG	C4-C3-C2	-4.21	104.69	111.23
4	K	201	NAG	C4-C3-C2	-3.71	105.46	111.23
4	E	202	NAG	C4-C3-C2	-3.33	106.05	111.23
4	Q	202	NAG	C3-C4-C5	-3.28	104.48	110.20
4	e	201	NAG	C4-C3-C2	-3.11	106.39	111.23
4	W	201	NAG	C4-C3-C2	-3.10	106.41	111.23
4	F	201	NAG	C6-C5-C4	-3.09	105.40	113.02
4	X	202	NAG	C3-C4-C5	-2.95	105.06	110.20
4	l	201	NAG	C2-N2-C7	-2.91	119.30	123.04
4	l	201	NAG	C3-C2-N2	-2.79	103.87	110.56
4	f	202	NAG	C3-C4-C5	-2.63	105.62	110.20
4	W	202	NAG	C2-N2-C7	-2.54	119.78	123.04
4	l	202	NAG	C2-N2-C7	-2.52	119.80	123.04
4	E	201	NAG	C2-N2-C7	-2.49	119.84	123.04
4	K	202	NAG	C3-C4-C5	-2.41	105.99	110.20
4	Q	202	NAG	C6-C5-C4	-2.40	107.09	113.02
4	R	202	NAG	C3-C4-C5	-2.38	106.04	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	202	NAG	C3-C4-C5	-2.38	106.05	110.20
4	Q	201	NAG	C2-N2-C7	-2.35	120.02	123.04
4	L	202	NAG	C3-C4-C5	-2.30	106.18	110.20
4	k	201	NAG	C2-N2-C7	-2.25	120.15	123.04
4	L	202	NAG	C3-C2-N2	-2.24	105.19	110.56
4	Q	202	NAG	C4-C3-C2	-2.24	107.75	111.23
4	F	202	NAG	C3-C4-C5	-2.18	106.41	110.20
4	f	201	NAG	C6-C5-C4	-2.05	107.96	113.02
4	X	202	NAG	O7-C7-C8	-2.03	118.33	122.06
4	k	201	NAG	C6-C5-C4	-2.03	108.01	113.02
4	l	201	NAG	C6-C5-C4	-2.03	108.01	113.02
4	W	202	NAG	C3-C4-C5	-2.02	106.67	110.20
4	W	202	NAG	C6-C5-C4	-2.01	108.06	113.02
4	X	202	NAG	C4-C3-C2	2.02	114.37	111.23
4	f	201	NAG	C3-C4-C5	2.03	113.74	110.20
4	l	201	NAG	C1-O5-C5	2.06	114.86	112.25
4	R	201	NAG	C3-C4-C5	2.07	113.81	110.20
4	F	201	NAG	O5-C5-C6	2.10	111.89	107.35
4	Q	201	NAG	O5-C5-C6	2.11	111.91	107.35
4	X	202	NAG	C1-O5-C5	2.14	114.97	112.25
4	e	201	NAG	O3-C3-C4	2.28	115.47	110.34
4	Q	201	NAG	C1-O5-C5	2.30	115.16	112.25
4	R	202	NAG	C2-N2-C7	2.34	126.05	123.04
4	e	202	NAG	C4-C3-C2	2.38	114.93	111.23
4	E	201	NAG	C3-C4-C5	2.40	114.38	110.20
4	X	202	NAG	C2-N2-C7	2.51	126.26	123.04
4	L	202	NAG	C1-O5-C5	2.54	115.48	112.25
4	K	202	NAG	C2-N2-C7	2.69	126.49	123.04
4	E	201	NAG	C1-O5-C5	2.92	115.95	112.25
4	K	202	NAG	O3-C3-C2	2.98	115.01	109.11
4	R	201	NAG	C4-C3-C2	3.01	115.90	111.23
4	F	201	NAG	C1-O5-C5	3.06	116.13	112.25
4	Q	202	NAG	O5-C5-C6	3.15	114.18	107.35
4	E	202	NAG	C2-N2-C7	3.37	127.36	123.04
4	f	202	NAG	C1-O5-C5	3.43	116.61	112.25
4	l	202	NAG	C1-O5-C5	3.44	116.62	112.25
4	X	201	NAG	C1-O5-C5	3.82	117.09	112.25
4	e	201	NAG	C1-O5-C5	4.63	118.12	112.25
4	W	202	NAG	C1-O5-C5	5.43	119.14	112.25
4	Q	202	NAG	C1-O5-C5	5.70	119.48	112.25
4	K	202	NAG	C1-O5-C5	5.83	119.65	112.25
4	K	201	NAG	C1-O5-C5	5.84	119.66	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	k	201	NAG	C1-O5-C5	6.05	119.92	112.25
4	E	202	NAG	C1-O5-C5	6.45	120.44	112.25

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	K	202	NAG	C1
4	X	202	NAG	C1
4	F	202	NAG	C1
4	l	202	NAG	C1
4	k	202	NAG	C1
4	L	202	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	202	NAG	O7-C7-N2-C2
4	E	202	NAG	O7-C7-N2-C2
4	X	201	NAG	O7-C7-N2-C2
4	l	202	NAG	O7-C7-N2-C2
4	l	202	NAG	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	201	NAG	4	0
4	K	202	NAG	2	0
4	L	201	NAG	1	0
4	L	202	NAG	2	0
4	Q	202	NAG	1	0
4	W	201	NAG	1	0
4	X	201	NAG	4	0
4	X	202	NAG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	105/110 (95%)	-0.46	0 100 100	35, 57, 90, 111	0
1	B	105/110 (95%)	-0.55	0 100 100	31, 60, 89, 111	0
1	G	105/110 (95%)	-0.53	0 100 100	34, 61, 90, 113	0
1	H	105/110 (95%)	-0.45	0 100 100	31, 59, 90, 110	0
1	M	105/110 (95%)	-0.46	0 100 100	39, 59, 90, 110	0
1	N	104/110 (94%)	-0.38	0 100 100	41, 65, 92, 124	0
1	S	105/110 (95%)	-0.43	0 100 100	32, 58, 89, 110	0
1	T	105/110 (95%)	-0.46	0 100 100	32, 59, 91, 112	0
1	a	105/110 (95%)	-0.46	0 100 100	39, 62, 97, 116	0
1	b	105/110 (95%)	-0.50	0 100 100	38, 62, 91, 111	0
1	g	105/110 (95%)	-0.42	0 100 100	36, 62, 92, 111	0
1	h	105/110 (95%)	-0.48	0 100 100	35, 60, 90, 110	0
2	C	75/106 (70%)	0.05	0 100 100	56, 94, 131, 160	0
2	D	72/106 (67%)	0.04	0 100 100	56, 96, 131, 161	0
2	I	75/106 (70%)	0.01	2 (2%) 58 58	59, 95, 131, 159	0
2	J	72/106 (67%)	0.03	1 (1%) 78 79	55, 95, 131, 161	0
2	O	75/106 (70%)	0.57	6 (8%) 15 15	64, 101, 141, 167	0
2	P	72/106 (67%)	-0.01	2 (2%) 56 57	58, 96, 130, 164	0
2	U	75/106 (70%)	0.07	3 (4%) 42 41	57, 95, 130, 160	0
2	V	72/106 (67%)	0.01	2 (2%) 56 57	60, 94, 131, 162	0
2	c	75/106 (70%)	0.22	2 (2%) 58 58	63, 99, 131, 159	0
2	d	72/106 (67%)	0.11	3 (4%) 40 39	58, 97, 131, 159	0
2	i	75/106 (70%)	0.24	0 100 100	62, 100, 131, 194	0
2	j	72/106 (67%)	0.03	2 (2%) 56 57	60, 97, 131, 162	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	E	91/124 (73%)	-0.07	0 100 100	48, 79, 120, 158	0
3	F	91/124 (73%)	-0.02	1 (1%) 82 83	56, 83, 121, 156	0
3	K	91/124 (73%)	-0.08	2 (2%) 65 65	63, 85, 124, 158	0
3	L	91/124 (73%)	-0.08	2 (2%) 65 65	45, 79, 119, 157	0
3	Q	91/124 (73%)	0.04	3 (3%) 50 50	46, 78, 118, 158	0
3	R	91/124 (73%)	0.34	6 (6%) 22 22	66, 92, 129, 185	0
3	W	91/124 (73%)	-0.06	1 (1%) 82 83	45, 78, 119, 158	0
3	X	91/124 (73%)	-0.04	2 (2%) 65 65	57, 82, 122, 158	0
3	e	91/124 (73%)	-0.02	0 100 100	63, 85, 122, 157	0
3	f	91/124 (73%)	-0.02	1 (1%) 82 83	43, 80, 121, 160	0
3	k	91/124 (73%)	-0.03	3 (3%) 50 50	58, 82, 122, 157	0
3	l	91/124 (73%)	-0.10	2 (2%) 65 65	44, 80, 120, 158	0
All	All	3233/4080 (79%)	-0.15	46 (1%) 78 79	31, 77, 124, 194	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	j	30	PRO	5.3
3	R	96	THR	4.7
2	P	30	PRO	3.7
2	O	48	GLY	3.5
3	L	34	GLU	3.4
2	V	30	PRO	3.2
2	P	98	ASN	3.1
2	j	31	LEU	3.1
3	R	51	THR	3.0
2	V	31	LEU	3.0
2	U	31	LEU	2.9
2	I	30	PRO	2.8
2	O	44	PRO	2.6
3	f	68	ASP	2.6
3	R	70	GLN	2.5
2	I	98	ASN	2.5
2	d	98	ASN	2.4
2	O	93	HIS	2.4
2	O	49	ALA	2.4
2	c	97	HIS	2.3
2	U	42	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	33	GLY	2.3
3	k	33	GLY	2.3
3	X	51	THR	2.3
2	U	30	PRO	2.2
2	d	44	PRO	2.2
3	R	41	CYS	2.2
2	J	93	HIS	2.2
3	l	98	LEU	2.2
3	Q	78	ASN	2.2
3	R	98	LEU	2.2
3	k	96	THR	2.2
3	k	98	LEU	2.2
3	F	35	GLN	2.1
2	d	33	THR	2.1
3	l	75	THR	2.1
3	K	35	GLN	2.1
3	X	68	ASP	2.1
3	K	98	LEU	2.1
3	Q	50	GLY	2.0
3	R	99	PRO	2.0
2	O	98	ASN	2.0
2	O	102	VAL	2.0
3	W	36	ASP	2.0
2	c	30	PRO	2.0
3	Q	34	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NA	e	203	1/1	0.87	0.33	2.92	52,52,52,52	0
5	NA	F	203	1/1	0.94	0.32	1.49	44,44,44,44	0
4	NAG	e	202	14/15	0.89	0.30	1.13	71,123,143,152	0
5	NA	K	203	1/1	0.93	0.27	0.60	36,36,36,36	0
4	NAG	W	202	14/15	0.92	0.25	0.10	28,84,111,118	0
4	NAG	E	202	14/15	0.90	0.23	0.06	42,101,122,123	0
4	NAG	X	202	14/15	0.93	0.24	-0.00	59,83,130,148	0
5	NA	k	203	1/1	0.90	0.23	-0.11	62,62,62,62	0
4	NAG	R	202	14/15	0.88	0.29	-0.16	69,118,135,152	0
5	NA	X	203	1/1	0.94	0.21	-0.19	37,37,37,37	0
4	NAG	L	202	14/15	0.91	0.25	-0.20	45,108,116,117	0
4	NAG	F	201	14/15	0.95	0.17	-0.23	57,72,98,98	0
4	NAG	f	202	14/15	0.89	0.27	-0.32	60,102,144,150	0
4	NAG	F	202	14/15	0.88	0.21	-0.43	84,107,120,127	0
4	NAG	R	201	14/15	0.95	0.16	-0.60	51,78,96,96	0
4	NAG	k	202	14/15	0.91	0.23	-0.63	47,105,157,168	0
4	NAG	e	201	14/15	0.97	0.14	-0.71	38,69,83,85	0
4	NAG	k	201	14/15	0.96	0.14	-0.73	55,77,95,97	0
4	NAG	l	202	14/15	0.91	0.18	-0.84	62,97,108,117	0
4	NAG	K	201	14/15	0.95	0.14	-0.85	43,82,92,93	0
4	NAG	Q	202	14/15	0.94	0.25	-0.88	29,77,96,102	0
4	NAG	K	202	14/15	0.91	0.20	-0.88	56,100,139,142	0
4	NAG	X	201	14/15	0.97	0.15	-0.89	30,61,82,92	0
4	NAG	L	201	14/15	0.97	0.14	-1.02	30,37,61,63	0
4	NAG	Q	201	14/15	0.97	0.14	-1.04	18,34,58,64	0
4	NAG	l	201	14/15	0.97	0.13	-1.15	18,36,51,65	0
4	NAG	f	201	14/15	0.98	0.14	-1.16	21,41,59,59	0
4	NAG	E	201	14/15	0.97	0.13	-1.30	28,41,56,67	0
5	NA	R	203	1/1	0.92	0.17	-1.50	58,58,58,58	0
4	NAG	W	201	14/15	0.97	0.13	-1.57	35,47,55,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.