



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:55 PM UTC

PDB ID : 7PA9 / pdb_00007pa9
Title : JC polyomavirus VP1 in complex with Fab 98D3
Authors : Stroeh, L.J.; Harprecht, C.; Freytag, J.; Stehle, T.
Deposited on : 2021-07-29
Resolution : 2.75 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

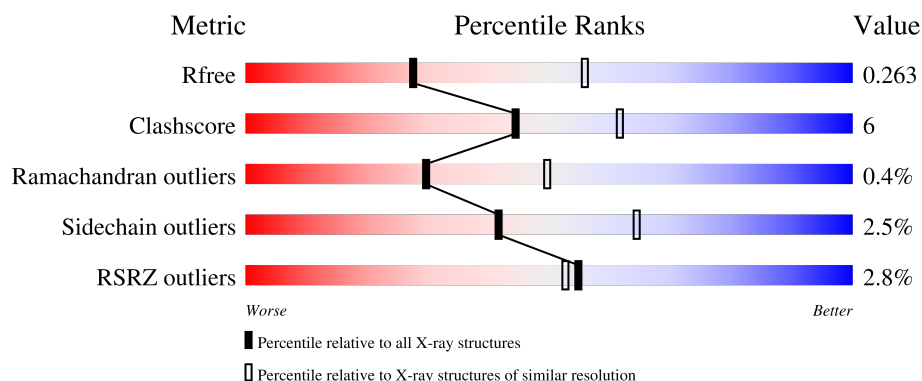
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



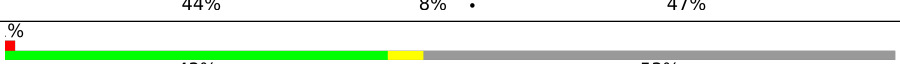
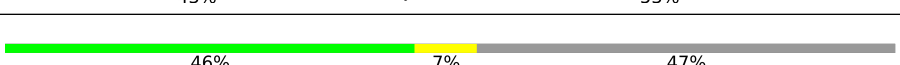
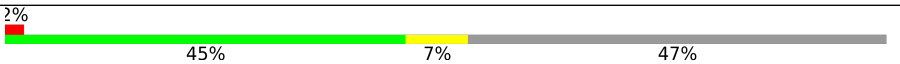
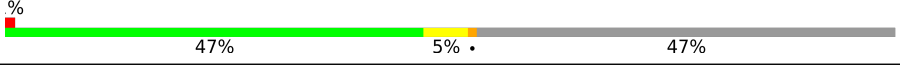
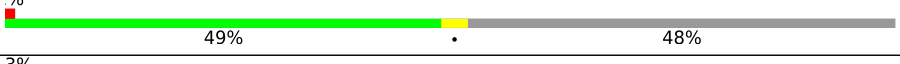
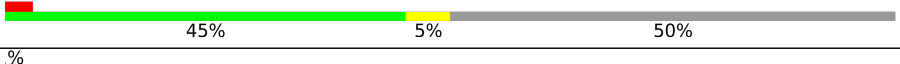
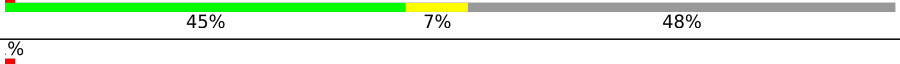
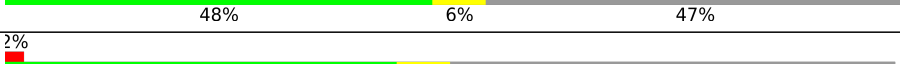
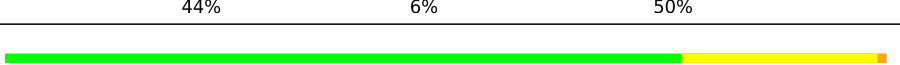
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	AAA	272	
1	BBB	272	
1	CCC	272	
1	DDD	272	
1	EEE	272	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	272	
1	GGG	272	
1	HHH	272	
1	III	272	
1	JJJ	272	
2	KKK	404	
2	MMM	404	
2	OOO	404	
2	QQQ	404	
2	TTT	404	
2	VVV	404	
2	XXX	404	
2	YYY	404	
2	bbb	404	
2	ccc	404	
3	LLL	212	
3	NNN	212	
3	PPP	212	
3	RRR	212	
3	SSS	212	
3	UUU	212	
3	WWW	212	
3	ZZZ	212	
3	aaa	212	
3	ddd	212	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51021 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	259	Total	C	N	O	S	0	0	0
			2014	1270	347	386	11			
1	BBB	258	Total	C	N	O	S	0	0	0
			2010	1269	344	386	11			
1	CCC	258	Total	C	N	O	S	0	0	0
			2009	1267	346	385	11			
1	DDD	259	Total	C	N	O	S	0	0	0
			2020	1274	347	388	11			
1	EEE	259	Total	C	N	O	S	0	0	0
			2023	1275	348	389	11			
1	FFF	259	Total	C	N	O	S	0	0	0
			2016	1272	347	386	11			
1	GGG	258	Total	C	N	O	S	0	0	0
			2015	1271	346	387	11			
1	HHH	258	Total	C	N	O	S	0	0	0
			2007	1264	345	387	11			
1	III	259	Total	C	N	O	S	0	0	0
			2016	1271	346	388	11			
1	JJJ	259	Total	C	N	O	S	0	0	0
			2018	1272	347	388	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression tag	UNP P03089
BBB	21	MET	-	expression tag	UNP P03089
CCC	18	GLY	-	expression tag	UNP P03089

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	19	SER	-	expression tag	UNP P03089
CCC	20	HIS	-	expression tag	UNP P03089
CCC	21	MET	-	expression tag	UNP P03089
DDD	18	GLY	-	expression tag	UNP P03089
DDD	19	SER	-	expression tag	UNP P03089
DDD	20	HIS	-	expression tag	UNP P03089
DDD	21	MET	-	expression tag	UNP P03089
EEE	18	GLY	-	expression tag	UNP P03089
EEE	19	SER	-	expression tag	UNP P03089
EEE	20	HIS	-	expression tag	UNP P03089
EEE	21	MET	-	expression tag	UNP P03089
FFF	18	GLY	-	expression tag	UNP P03089
FFF	19	SER	-	expression tag	UNP P03089
FFF	20	HIS	-	expression tag	UNP P03089
FFF	21	MET	-	expression tag	UNP P03089
GGG	18	GLY	-	expression tag	UNP P03089
GGG	19	SER	-	expression tag	UNP P03089
GGG	20	HIS	-	expression tag	UNP P03089
GGG	21	MET	-	expression tag	UNP P03089
HHH	18	GLY	-	expression tag	UNP P03089
HHH	19	SER	-	expression tag	UNP P03089
HHH	20	HIS	-	expression tag	UNP P03089
HHH	21	MET	-	expression tag	UNP P03089
III	18	GLY	-	expression tag	UNP P03089
III	19	SER	-	expression tag	UNP P03089
III	20	HIS	-	expression tag	UNP P03089
III	21	MET	-	expression tag	UNP P03089
JJJ	18	GLY	-	expression tag	UNP P03089
JJJ	19	SER	-	expression tag	UNP P03089
JJJ	20	HIS	-	expression tag	UNP P03089
JJJ	21	MET	-	expression tag	UNP P03089

- Molecule 2 is a protein called Fab 98D3 VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	KKK	214	Total	C	N	O	S	0	0	0
			1599	1013	268	313	5			
2	MMM	191	Total	C	N	O	S	0	0	0
			1401	886	236	274	5			
2	OOO	215	Total	C	N	O	S	0	0	0
			1593	1011	267	310	5			
2	QQQ	213	Total	C	N	O	S	0	0	0
			1561	987	259	310	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	TTT	214	Total	C	N	O	S	0	0	0
			1575	996	264	310	5			
2	VVV	212	Total	C	N	O	S	0	0	0
			1579	1004	264	306	5			
2	XXX	203	Total	C	N	O	S	0	0	0
			1500	955	249	291	5			
2	YYY	212	Total	C	N	O	S	0	0	0
			1584	1004	267	308	5			
2	bbb	215	Total	C	N	O	S	0	0	0
			1588	1008	264	311	5			
2	ccc	202	Total	C	N	O	S	0	0	0
			1503	958	250	290	5			

- Molecule 3 is a protein called Fab 98D3 VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	LLL	211	Total	C	N	O	S	0	0	0
			1592	993	266	328	5			
3	NNN	157	Total	C	N	O	S	0	0	0
			1160	728	183	245	4			
3	PPP	211	Total	C	N	O	S	0	0	0
			1570	977	263	325	5			
3	RRR	202	Total	C	N	O	S	0	0	0
			1515	947	249	314	5			
3	SSS	199	Total	C	N	O	S	0	0	0
			1493	930	248	310	5			
3	UUU	175	Total	C	N	O	S	0	0	0
			1328	831	221	272	4			
3	WWW	212	Total	C	N	O	S	0	0	0
			1605	1000	270	330	5			
3	ZZZ	211	Total	C	N	O	S	0	0	0
			1614	1010	270	329	5			
3	aaa	211	Total	C	N	O	S	0	0	0
			1595	994	267	329	5			
3	ddd	206	Total	C	N	O	S	0	0	0
			1572	983	263	321	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	22	Total	O	0	0
			22	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	31	Total 31	O 31	0	0
4	CCC	27	Total 27	O 27	0	0
4	DDD	23	Total 23	O 23	0	0
4	EEE	29	Total 29	O 29	0	0
4	FFF	22	Total 22	O 22	0	0
4	GGG	35	Total 35	O 35	0	0
4	HHH	34	Total 34	O 34	0	0
4	III	31	Total 31	O 31	0	0
4	JJJ	31	Total 31	O 31	0	0
4	KKK	9	Total 9	O 9	0	0
4	LLL	9	Total 9	O 9	0	0
4	MMM	4	Total 4	O 4	0	0
4	NNN	2	Total 2	O 2	0	0
4	OOO	3	Total 3	O 3	0	0
4	PPP	3	Total 3	O 3	0	0
4	QQQ	6	Total 6	O 6	0	0
4	RRR	4	Total 4	O 4	0	0
4	SSS	3	Total 3	O 3	0	0
4	TTT	2	Total 2	O 2	0	0
4	UUU	2	Total 2	O 2	0	0
4	VVV	3	Total 3	O 3	0	0

Continued on next page...

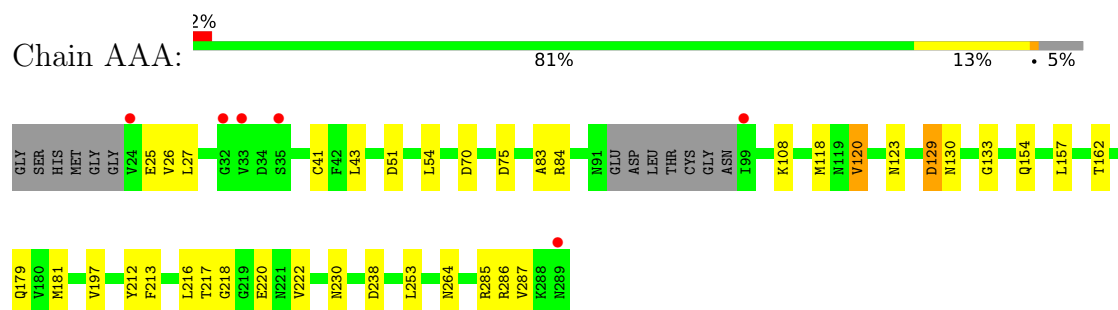
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	WWW	1	Total	O	0	0
			1	1		
4	XXX	1	Total	O	0	0
			1	1		
4	YYY	1	Total	O	0	0
			1	1		
4	ZZZ	1	Total	O	0	0
			1	1		
4	bbb	1	Total	O	0	0
			1	1		
4	ccc	4	Total	O	0	0
			4	4		
4	ddd	2	Total	O	0	0
			2	2		

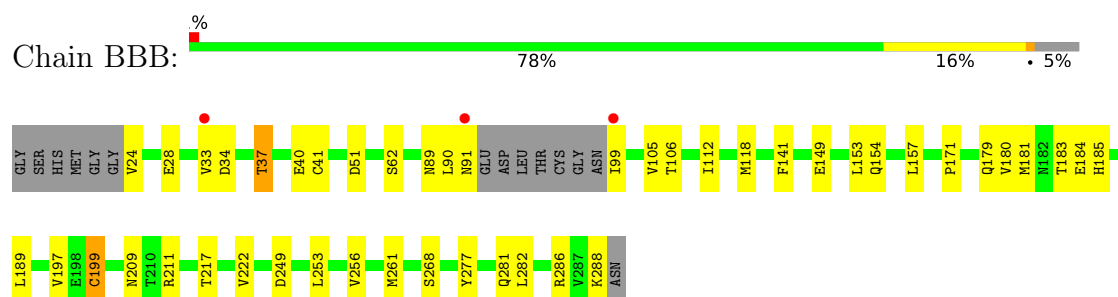
3 Residue-property plots [i](#)

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.

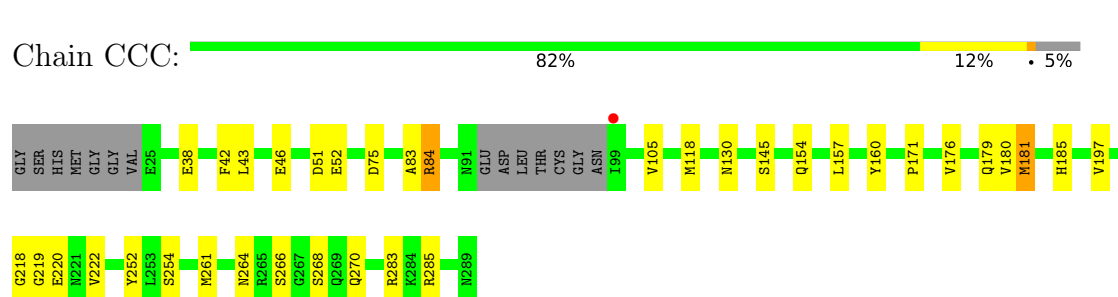
- Molecule 1: Major capsid protein VP1



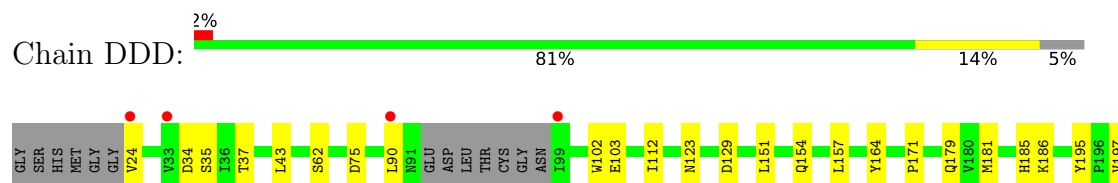
- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1

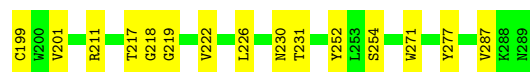
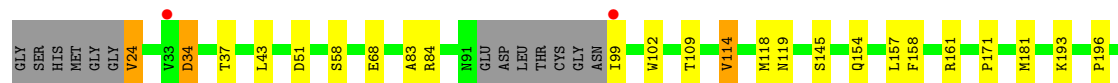
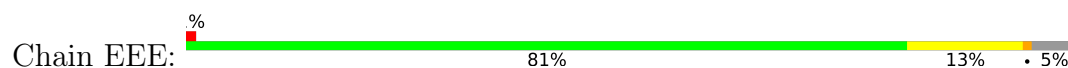


- Molecule 1: Major capsid protein VP1

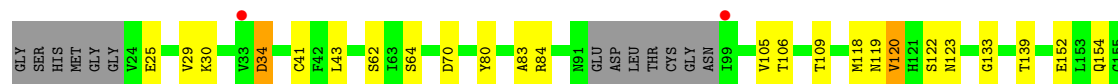
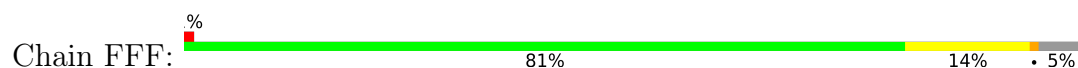




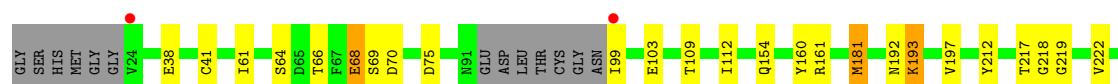
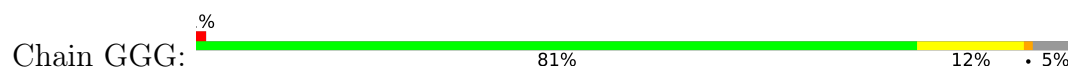
- Molecule 1: Major capsid protein VP1



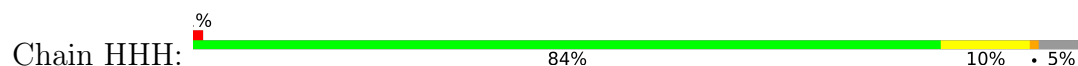
- Molecule 1: Major capsid protein VP1



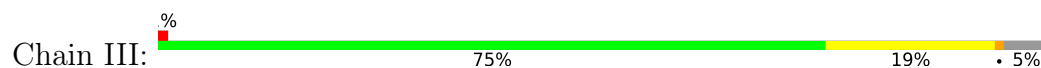
- Molecule 1: Major capsid protein VP1

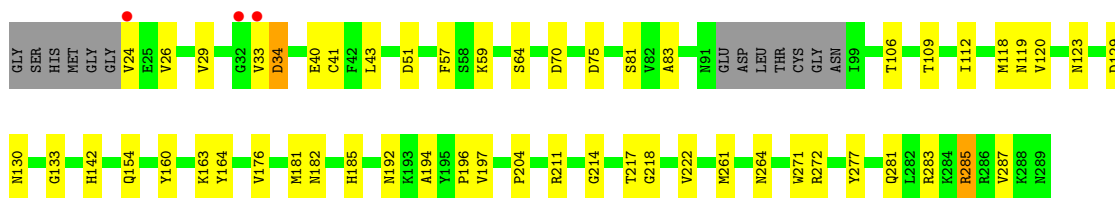


- Molecule 1: Major capsid protein VP1

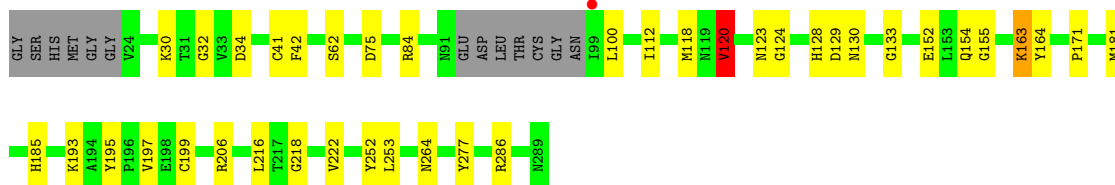
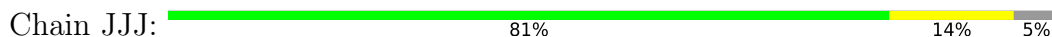


- Molecule 1: Major capsid protein VP1

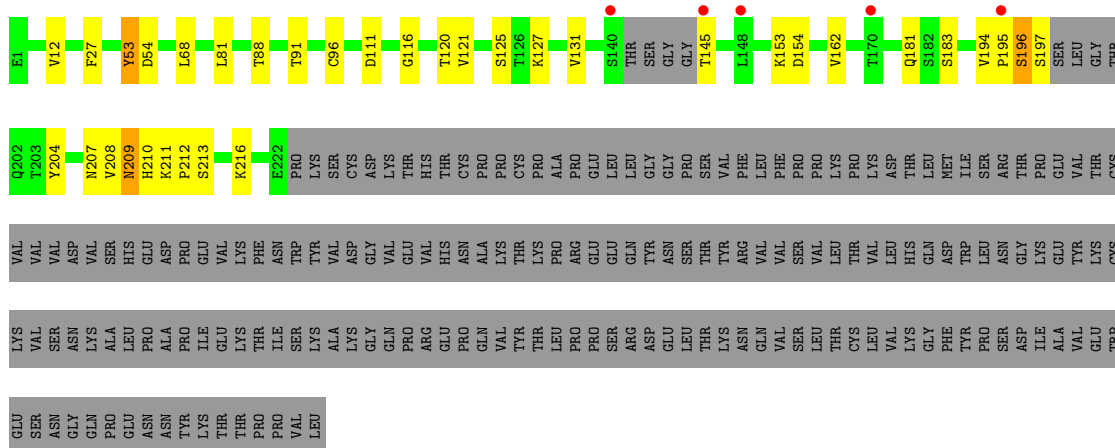




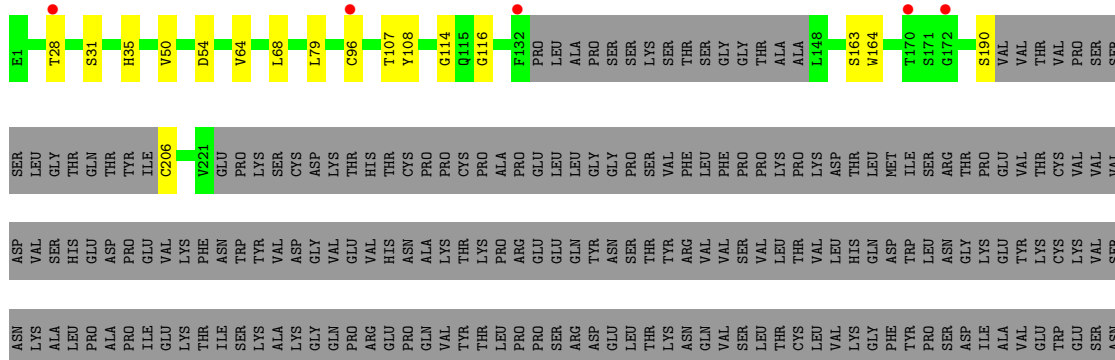
- Molecule 1: Major capsid protein VP1



- Molecule 2: Fab 98D3 VH



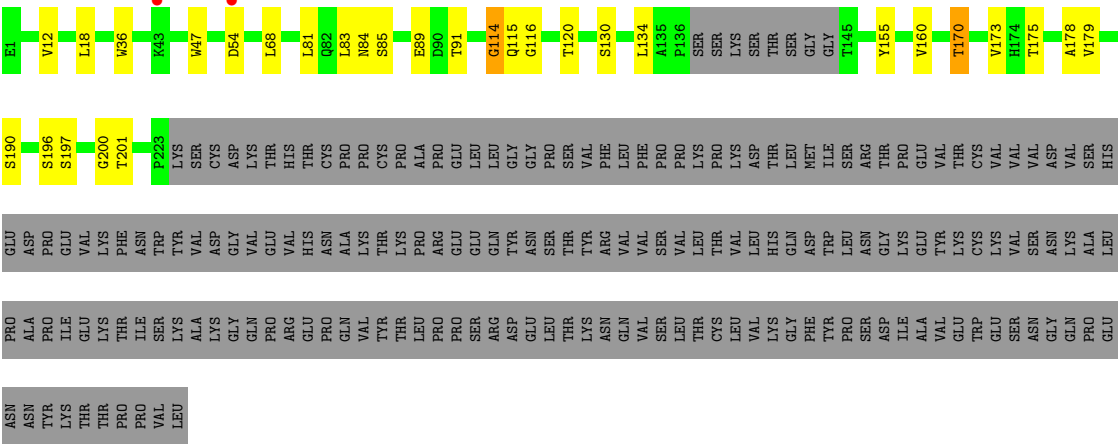
- Molecule 2: Fab 98D3 VH



GLY
GLN
PRO
GLU
ASN
TYR
THR
PRO
PRO
VAL
LEU

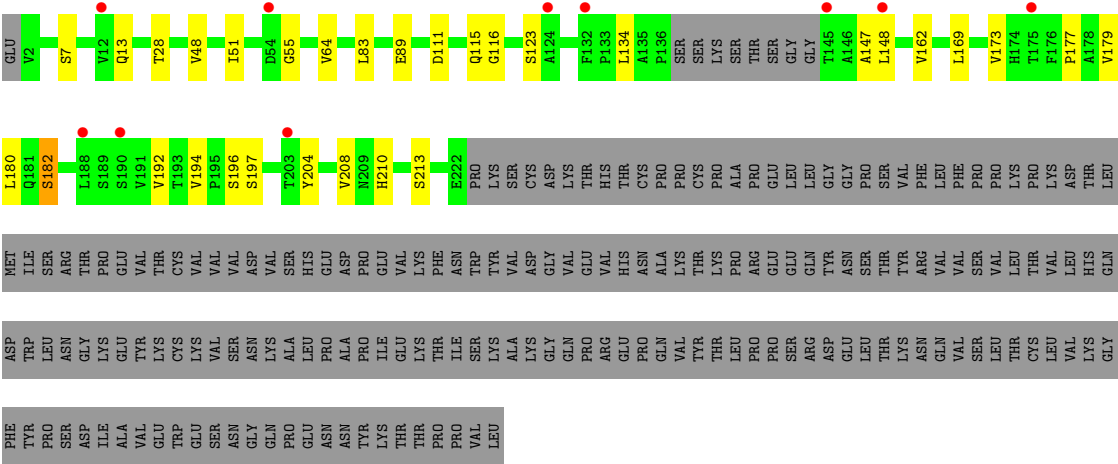
● Molecule 2: Fab 98D3 VH

Chain OOO: 46% 7% 47%



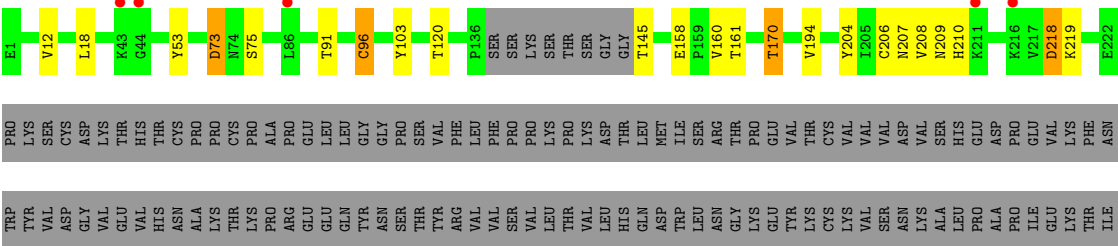
● Molecule 2: Fab 98D3 VH

Chain QQQ: 2% 45% 7% 47%



● Molecule 2: Fab 98D3 VH

Chain TTT: 47% 5% 47%



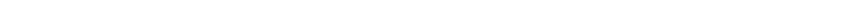
[illegible]

- Molecule 2: Fab 98D3 VH

Chain VVV:

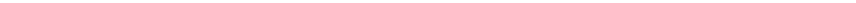
[illegible]

- Molecule 2: Fab 98D3 VH

Chain XXX: 

[illegible]

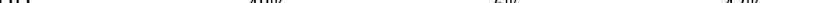
- Molecule 2: Fab 98D3 VH

Chain YYY:  %

Residue	Position	Sequence	Structure	Function
GLU	V2	GLU	GLU	GLU
F27	F27	ASP	ASP	ASP
Y53	K211	PRO	PRO	PRO
D54	P212	GLU	GLU	GLU
S71	V217	VAL	VAL	VAL
Y80	E222	LYS	LYS	LYS
T88	P80	ASN	ASN	ASN
T91	TRP	TRP	TRP	TRP
R98	TYR	TYR	TYR	TYR
D111	VAL	VAL	VAL	VAL
F112	HIS	HIS	HIS	HIS
V121	ASN	ASN	ASN	ASN
K127	ALA	ALA	ALA	ALA
V131	LYS	LYS	LYS	LYS
F132	PRO	PRO	PRO	PRO
P133	ARG	ARG	ARG	ARG
L134	GLU	GLU	GLU	GLU
A135	LEU	LEU	LEU	LEU
P136	GLN	GLN	GLN	GLN
SER	TYR	TYR	TYR	TYR
SER	ASN	ASN	ASN	ASN
SER	SER	SER	SER	SER
SER	THR	THR	THR	THR
SER	VAL	VAL	VAL	VAL
SER	ARG	ARG	ARG	ARG
SER	VAL	VAL	VAL	VAL
SER	VAL	VAL	VAL	VAL
SER	VAL	VAL	VAL	VAL
SER	LEU	LEU	LEU	LEU
SER	LEU	LEU	LEU	LEU
SER	THR	THR	THR	THR
SER	VAL	VAL	VAL	VAL
SER	LEU	LEU	LEU	LEU
SER	THR	THR	THR	THR
SER	LYS	LYS	LYS	LYS
SER	ASP	ASP	ASP	ASP
SER	THR	THR	THR	THR
SER	MET	MET	MET	MET
SER	ILE	ILE	ILE	ILE
SER	SER	SER	SER	SER
SER	ARG	ARG	ARG	ARG
SER	THR	THR	THR	THR
SER	PRO	PRO	PRO	PRO
SER	VAL	VAL	VAL	VAL
SER	THR	THR	THR	THR
SER	LYS	LYS	LYS	LYS
SER	VAL	VAL	VAL	VAL
SER	LEU	LEU	LEU	LEU
SER	THR	THR	THR	THR
SER	LYS	LYS	LYS	LYS
SER	CYS	CYS	CYS	CYS
SER	VAL	VAL	VAL	VAL
SER	VAL	VAL	VAL	VAL
SER	VAL	VAL	VAL	VAL
SER	ASN	ASN	ASN	ASN
SER	LYS	LYS	LYS	LYS

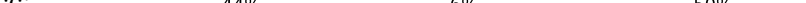
[illegible]

- Molecule 2: Fab 98D3 VH

Chain bbb: 

LYS	GLN	GLY	ASP	GLY	GLN	ASP	CYS	E1
GLN	GLY	VAL	GLY	VAL	GLY	ASP	LYS	V2
PRO	ARG	GLU	VAL	GLU	THR	THR	HIS	V48
GLU	GLU	HIS	ASN	THR	THR	THR	THR	V64
GLN	VAL	ASN	ALA	ALA	CYS	CYS	CYS	L68
VAL	VAL	LYS	THR	THR	PRO	PRO	PRO	D73
THR	THR	LYS	THR	LYS	PRO	PRO	PRO	N74
LEU	LEU	PRO	ARG	ALA	ALA	ALA	ALA	S75
PRO	PRO	ARG	GLY	GLY	PRO	PRO	PRO	C96
PRO	PRO	GLU	GLU	GLU	GLU	GLU	LEU	G102
ARG	ARG	GLN	GLN	GLY	LEU	LEU	LEU	Y103
ASP	ASP	TYR	ASN	GLY	GLY	GLY	GLY	Q115
LEU	LEU	SER	SER	SER	PRO	PRO	PRO	G116
THR	THR	THR	THR	THR	SER	SER	SER	T120
LYS	LYS	TYR	VAL	VAL	PHE	PHE	PHE	T120
ASN	ASN	ARG	ARG	VAL	VAL	PHE	PHE	F132
GLN	GLN	VAL	VAL	VAL	VAL	VAL	VAL	P133
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	L134
SER	SER	SER	SER	SER	PRO	PRO	PRO	A135
LYS	LYS	LEU	LEU	LEU	VAL	VAL	VAL	P136
THR	THR	LEU	LEU	LEU	VAL	VAL	VAL	SER
CYS	CYS	THR	THR	THR	THR	THR	THR	SER
LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	SER
VAL	VAL	LEU	LEU	LEU	LEU	LEU	LEU	LYS
VAL	VAL	LEU	LEU	LEU	LEU	LEU	LEU	LYS
LYS	LYS	HIS	HIS	HIS	THR	THR	THR	LYS
GLY	GLY	GLN	GLN	GLN	LEU	LEU	LEU	SER
PHE	PHE	ASP	ASP	ASP	MET	MET	THR	THR
TYR	TYR	TRP	TRP	TRP	ILE	ILE	SER	SER
PRO	PRO	LEU	LEU	LEU	SER	SER	GLY	GLY
SER	SER	ASN	ASN	ASN	ARG	ARG	ARG	GLY
ASP	ASP	GLY	GLY	GLY	THR	THR	THR	T145
ILE	ILE	LYS	LYS	LYS	PRO	PRO	PRO	T170
ALA	ALA	GLU	GLU	GLU	GLU	GLU	GLU	S171
VAL	VAL	TYR	TYR	TYR	VAL	VAL	THR	G172
GLU	GLU	LYS	LYS	LYS	CYS	CYS	CYS	L180
TRP	TRP	CYS	CYS	CYS	VAL	VAL	VAL	Q181
GLU	GLU	LYS	LYS	LYS	VAL	VAL	VAL	L185
GLY	GLY	ASN	ASN	ASN	ASP	ASP	ASP	V192
PRO	PRO	LYS	LYS	LYS	VAL	VAL	VAL	S196
PRO	PRO	ALA	ALA	ALA	SER	SER	SER	S197
ASN	ASN	PRO	PRO	PRO	GLU	GLU	GLU	S198
VAL	VAL	THR	THR	THR	PRO	PRO	PRO	T203
LEU	LEU	ILE	ILE	ILE	GLU	GLU	VAL	M214
VAL	VAL	THR	THR	THR	VAL	VAL	VAL	P223
VAL	VAL	THR	THR	THR	THR	THR	THR	LYS
LEU	LEU	ALA	ALA	ALA	VAL	VAL	VAL	SER

- Molecule 2: Fab 98D3 VH

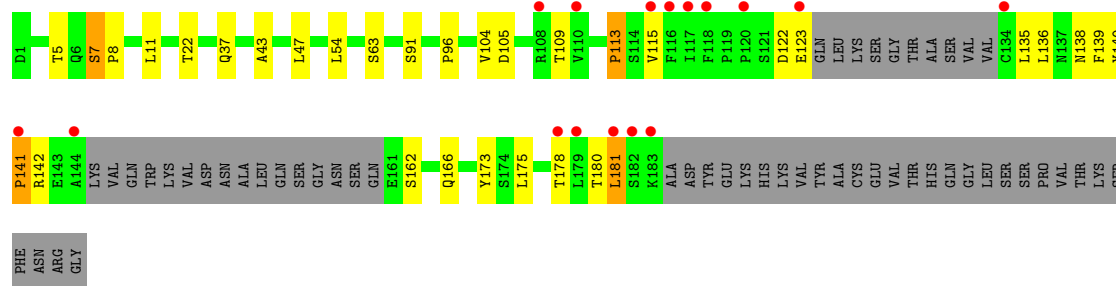
Chain ccc: 

SER	ASN	ARG	T193	E1
ASP	GLY	THR	V194	
ILE	LYS	PRO	P195	S21
ALA	GLU	GLU	SER	
VAL	TYR	VAL	SER	F27
GLU	LYS	THR	SER	
TRP	CYS	LEU	LEU	M34
GLU	LYS	VAL	GLY	
TRP	VAL	THR	THR	
SER	VAL	VAL	GLN	Y53
ASN	SER	VAL	THR	D54
GLY	ASN	ASP	THR	
GLN	LYS	VAL	Y204	V64
PRO	ALA	SER		
GLU	LEU	HIS	N207	R67
ASN	PRO	GLU		L68
TYR	ALA	ASP	K211	
ASN	PRO	PRO	P212	D73
LYS	ILE	GLU		M74
GLU	GLY	VAL	D218	S75
THR	LYS	LYS		
THR	THR	PHE	V221	L79
PRO	PRO	ILE	GLU	
PRO	LYS	THR	PRO	L83
VAL	LYS	TYR	LYS	
LEU	ALA	VAL	SER	R98
	LYS	ASP	CYS	
	GLY	GLY	ASP	G116
	GLN	VAL	LYS	
	PRO	GLU	THR	T120
	ARG	VAL	HIS	
	GLU	HIS	THR	S125
	PRO	ASN	CYS	
	GLN	ALA	PRO	P129
	VAL	LYS	PRO	
	TYR	THR	CYS	A135
	THR	LYS	PRO	
	LEU	PRO	ALA	PRO
	PRO	ARG	SER	SER
	PRO	GLU	GLU	LYS
	SER	GLU	LEU	SER
	ARG	GLN	LEU	THR
	ASP	TYR	GLY	SER
	GLU	ASN	GLY	GLY
	LEU	SER	PRO	THR
	THR	THR	SER	VAL
	LYS	TYR	VAL	ALA
	ASN	ARG	PHE	A147
	GLN	VAL	LEU	L148
	VAL	VAL	PHE	
	SER	SER	PRO	Y155
	LEU	VAL	PRO	
	THR	LEU	LYS	T170
	CYS	THR	PRO	
	LEU	VAL	LYS	V173
	VAL	LEU	ASP	
	LYS	HIS	THR	Q181
	GLY	GLN	LEU	
	PHE	ASP	MET	L185
	PRO	THR	ILE	
	PRO	LEU	SER	V193

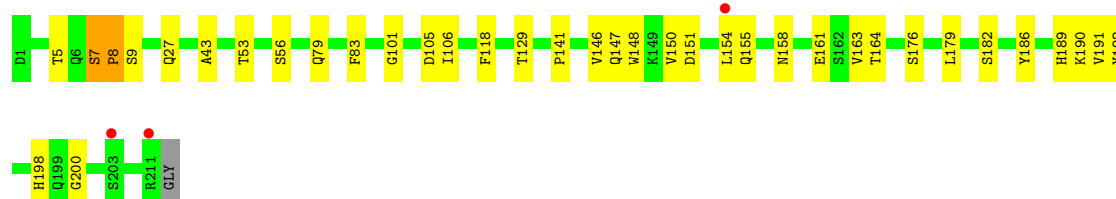
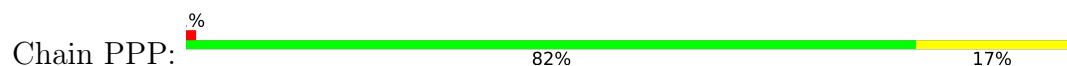
- Molecule 3: Fab 98D3 VL

Chain LLL: 76% 22%

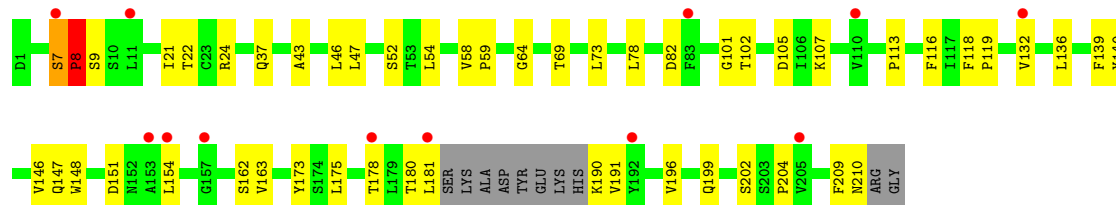
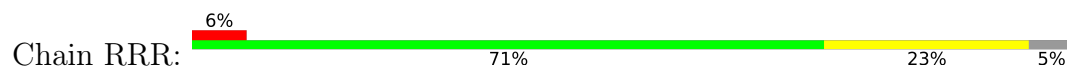
- Molecule 3: Fab 98D3 VL



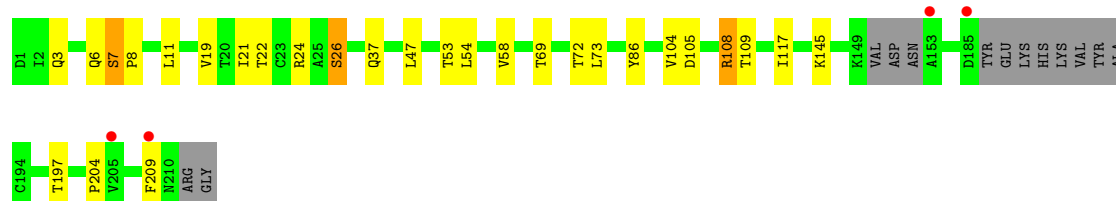
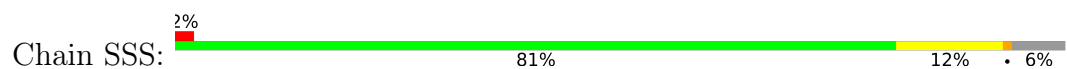
- Molecule 3: Fab 98D3 VL



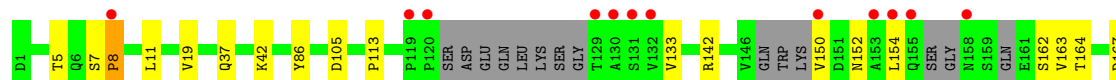
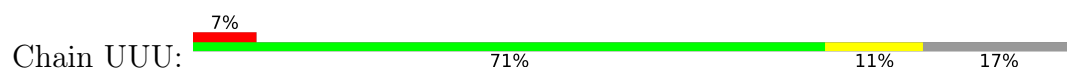
- Molecule 3: Fab 98D3 VL

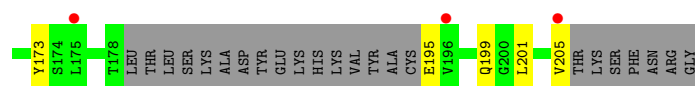


- Molecule 3: Fab 98D3 VL

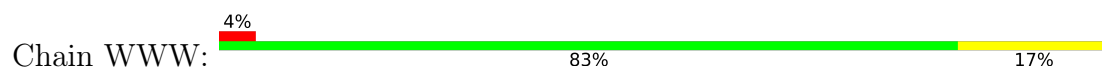


- Molecule 3: Fab 98D3 VL

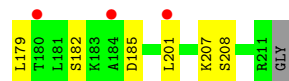
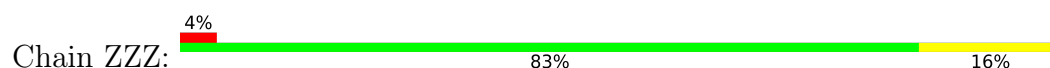




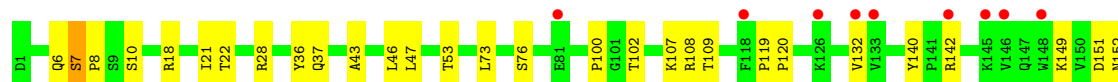
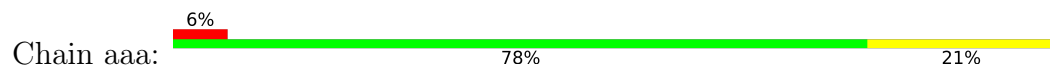
• Molecule 3: Fab 98D3 VL



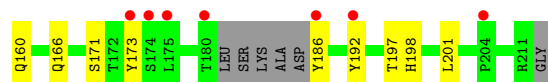
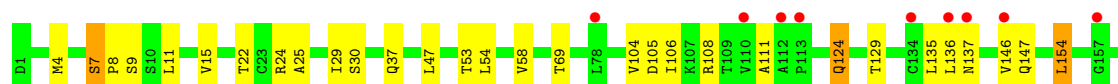
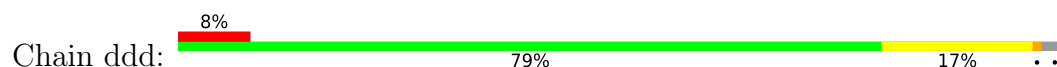
• Molecule 3: Fab 98D3 VL



• Molecule 3: Fab 98D3 VL



• Molecule 3: Fab 98D3 VL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.97Å 202.31Å 251.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.75 49.15 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.75) 100.0 (49.15-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.207 , 0.263 0.210 , 0.263	Depositor DCC
R_{free} test set	11285 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	51021	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	1.01	0/2059	1.37	4/2797 (0.1%)
1	BBB	1.00	0/2055	1.37	2/2792 (0.1%)
1	CCC	0.99	0/2054	1.36	4/2790 (0.1%)
1	DDD	0.98	0/2065	1.37	8/2805 (0.3%)
1	EEE	1.00	0/2068	1.33	3/2809 (0.1%)
1	FFF	0.99	0/2061	1.36	4/2800 (0.1%)
1	GGG	0.97	0/2060	1.36	5/2798 (0.2%)
1	HHH	0.98	0/2052	1.36	3/2788 (0.1%)
1	III	0.99	0/2061	1.35	2/2801 (0.1%)
1	JJJ	1.01	0/2063	1.38	8/2802 (0.3%)
2	KKK	1.02	0/1636	1.38	4/2227 (0.2%)
2	MMM	1.07	0/1434	1.37	1/1956 (0.1%)
2	OOO	1.03	0/1632	1.34	6/2227 (0.3%)
2	QQQ	1.04	0/1599	1.33	5/2190 (0.2%)
2	TTT	1.06	0/1612	1.43	5/2200 (0.2%)
2	VVV	1.03	0/1618	1.35	0/2207
2	XXX	1.04	0/1536	1.36	2/2096 (0.1%)
2	YYY	1.03	0/1622	1.37	3/2211 (0.1%)
2	bbb	1.03	0/1627	1.36	4/2222 (0.2%)
2	ccc	1.06	0/1539	1.41	5/2097 (0.2%)
3	LLL	1.03	0/1628	1.38	6/2221 (0.3%)
3	NNN	1.09	0/1186	1.44	2/1622 (0.1%)
3	PPP	1.06	1/1606 (0.1%)	1.38	3/2197 (0.1%)
3	RRR	1.08	1/1548 (0.1%)	1.40	7/2113 (0.3%)
3	SSS	1.07	0/1524	1.38	3/2076 (0.1%)
3	UUU	1.03	0/1353	1.36	3/1837 (0.2%)
3	WWW	1.07	0/1641	1.40	2/2234 (0.1%)
3	ZZZ	1.05	0/1650	1.34	0/2243
3	aaa	1.05	0/1629	1.40	2/2216 (0.1%)
3	ddd	1.10	0/1607	1.43	3/2185 (0.1%)
All	All	1.03	2/51825 (0.0%)	1.37	109/70559 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	RRR	8	PRO	C-O	-5.52	1.16	1.24
3	PPP	79	GLN	N-CA	5.46	1.49	1.46

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	RRR	8	PRO	CA-N-CD	-7.73	101.18	112.00
1	HHH	32	GLY	CA-C-O	-7.48	117.07	122.23
1	CCC	219	GLY	CA-C-O	-7.25	117.51	122.22
3	LLL	53	THR	CA-CB-OG1	-7.21	98.78	109.60
2	ccc	53	TYR	CA-C-N	6.93	131.22	120.82
2	ccc	53	TYR	C-N-CA	6.93	131.22	120.82
1	BBB	33	VAL	N-CA-C	-6.86	106.45	113.10
1	DDD	129	ASP	CB-CA-C	6.75	119.88	110.16
1	JJJ	193	LYS	CB-CA-C	-6.71	100.82	111.48
1	CCC	75	ASP	CA-CB-CG	6.68	119.28	112.60
3	RRR	101	GLY	CA-C-O	-6.58	117.69	122.23
2	bbb	116	GLY	CA-C-O	-6.51	117.74	122.23
1	III	75	ASP	CA-CB-CG	6.42	119.02	112.60
3	RRR	8	PRO	CB-CA-C	6.37	122.07	111.56
1	JJJ	75	ASP	CA-CB-CG	6.32	118.92	112.60
3	ddd	53	THR	CB-CA-C	6.31	120.88	110.78
1	GGG	75	ASP	CA-CB-CG	6.30	118.90	112.60
3	PPP	8	PRO	N-CA-C	-6.27	101.33	110.80
3	RRR	8	PRO	N-CA-CB	-6.16	96.78	103.25
2	ccc	54	ASP	CB-CA-C	-6.04	100.72	110.74
1	JJJ	164	TYR	CB-CA-C	6.03	118.12	109.26
3	aaa	53	THR	CA-CB-OG1	-6.01	100.58	109.60
3	UUU	8	PRO	N-CA-C	-5.92	100.28	112.47
3	WWW	53	THR	CA-CB-OG1	-5.88	100.78	109.60
1	DDD	265	ARG	CA-C-N	5.85	128.39	120.38
1	DDD	265	ARG	C-N-CA	5.85	128.39	120.38
2	YYY	53	TYR	CA-C-N	5.83	129.56	120.82
2	YYY	53	TYR	C-N-CA	5.83	129.56	120.82
3	SSS	104	VAL	CA-C-N	5.82	131.37	122.93
3	SSS	104	VAL	C-N-CA	5.82	131.37	122.93
1	JJJ	120	VAL	N-CA-C	-5.81	105.72	111.88
1	JJJ	195	TYR	CB-CA-C	5.75	116.69	110.08
2	YYY	54	ASP	CB-CA-C	-5.74	101.22	110.74
1	DDD	164	TYR	CB-CA-C	5.73	118.50	109.27
1	III	164	TYR	CB-CA-C	5.70	117.06	108.86
1	AAA	120	VAL	N-CA-CB	-5.67	104.57	111.94
1	DDD	202	PRO	CA-C-O	-5.64	115.17	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	ddd	104	VAL	CA-C-N	5.63	130.43	122.09
3	ddd	104	VAL	C-N-CA	5.63	130.43	122.09
2	ccc	64	VAL	CA-C-O	-5.63	115.07	119.46
2	TTT	53	TYR	CA-C-N	5.60	129.23	120.82
2	TTT	53	TYR	C-N-CA	5.60	129.23	120.82
1	DDD	90	LEU	N-CA-C	-5.60	100.76	109.72
2	OOO	47	TRP	CA-C-N	5.56	128.69	123.08
2	OOO	47	TRP	C-N-CA	5.56	128.69	123.08
1	EEE	114	VAL	CA-C-O	-5.55	114.63	120.57
2	MMM	116	GLY	CA-C-O	-5.53	118.42	122.23
1	EEE	219	GLY	CA-C-O	-5.53	117.57	121.88
1	GGG	193	LYS	CB-CA-C	-5.52	100.63	111.06
3	SSS	53	THR	CA-CB-OG1	-5.51	101.33	109.60
2	bbb	196	SER	CA-C-N	5.49	127.90	120.38
2	bbb	196	SER	C-N-CA	5.49	127.90	120.38
3	LLL	199	GLN	CA-C-N	5.48	125.92	119.94
3	LLL	199	GLN	C-N-CA	5.48	125.92	119.94
2	ccc	116	GLY	CA-C-O	-5.48	118.50	122.45
1	FFF	120	VAL	N-CA-CB	-5.45	102.25	111.23
3	RRR	64	GLY	CA-C-O	-5.41	116.86	121.57
1	DDD	195	TYR	CB-CA-C	5.40	116.29	110.08
1	FFF	193	LYS	CB-CA-C	-5.40	102.56	111.36
3	aaa	28	ARG	CB-CA-C	5.35	118.46	109.89
1	DDD	75	ASP	CA-CB-CG	5.34	117.94	112.60
3	PPP	101	GLY	CA-C-O	-5.33	117.97	122.29
1	JJJ	32	GLY	CA-C-O	-5.32	118.76	122.22
2	OOO	114	GLY	CA-C-N	5.31	127.93	120.28
2	OOO	114	GLY	C-N-CA	5.31	127.93	120.28
3	PPP	8	PRO	CB-CA-C	5.31	117.88	111.46
2	KKK	53	TYR	CA-C-N	5.30	128.78	120.82
2	KKK	53	TYR	C-N-CA	5.30	128.78	120.82
2	TTT	96	CYS	CB-CA-C	5.28	118.46	109.80
1	AAA	75	ASP	CA-CB-CG	5.27	117.87	112.60
1	FFF	152	GLU	CB-CA-C	5.26	118.43	109.80
3	LLL	141	PRO	CA-C-N	5.26	127.64	120.54
3	LLL	141	PRO	C-N-CA	5.26	127.64	120.54
2	KKK	116	GLY	CA-C-O	-5.25	117.73	122.57
3	WWW	20	THR	CA-CB-OG1	-5.25	101.73	109.60
1	GGG	68	GLU	CB-CG-CD	5.25	121.52	112.60
3	RRR	59	PRO	CA-C-N	5.24	128.99	120.60
3	RRR	59	PRO	C-N-CA	5.24	128.99	120.60
2	OOO	200	GLY	CA-C-N	5.23	127.28	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	OOO	200	GLY	C-N-CA	5.23	127.28	120.28
1	HHH	219	GLY	CA-C-O	-5.21	117.81	121.88
3	NNN	113	PRO	CB-CA-C	-5.19	106.68	111.40
1	CCC	46	GLU	CB-CA-C	5.18	119.47	111.95
1	GGG	234	THR	CA-CB-OG1	-5.18	101.82	109.60
1	BBB	28	GLU	N-CA-C	5.18	117.22	110.43
1	HHH	175	THR	CA-CB-OG1	-5.17	101.84	109.60
2	XXX	28	THR	CA-C-N	5.14	128.53	120.82
2	XXX	28	THR	C-N-CA	5.14	128.53	120.82
1	JJJ	120	VAL	N-CA-CB	-5.14	105.26	111.94
1	AAA	238	ASP	CA-C-N	5.14	128.90	120.63
1	AAA	238	ASP	C-N-CA	5.14	128.90	120.63
2	TTT	218	ASP	CB-CA-C	5.12	118.57	109.72
1	EEE	119	ASN	N-CA-CB	5.11	117.72	110.46
2	bbb	120	THR	CB-CA-C	5.11	118.55	109.72
1	FFF	120	VAL	CB-CA-C	5.09	119.64	111.29
1	GGG	219	GLY	CA-C-O	-5.09	117.81	122.24
2	QQQ	116	GLY	CA-C-O	-5.06	118.52	122.52
2	QQQ	196	SER	CA-C-N	5.06	127.02	120.44
2	QQQ	196	SER	C-N-CA	5.06	127.02	120.44
1	JJJ	124	GLY	CA-C-O	-5.06	116.32	120.92
2	QQQ	182	SER	CA-C-N	5.06	127.31	120.38
2	QQQ	182	SER	C-N-CA	5.06	127.31	120.38
2	TTT	170	THR	CA-CB-OG1	-5.02	102.07	109.60
1	CCC	38	GLU	CB-CA-C	5.02	119.87	109.38
3	LLL	101	GLY	CA-C-O	-5.02	117.46	121.77
3	UUU	167	ASP	CA-C-N	5.01	127.24	120.38
3	UUU	167	ASP	C-N-CA	5.01	127.24	120.38
2	KKK	27	PHE	CA-CB-CG	5.00	118.80	113.80
3	NNN	5	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2014	0	1965	42	0
1	BBB	2010	0	1963	32	0
1	CCC	2009	0	1963	22	0
1	DDD	2020	0	1976	23	0
1	EEE	2023	0	1980	30	0
1	FFF	2016	0	1972	31	0
1	GGG	2015	0	1974	26	0
1	HHH	2007	0	1949	19	0
1	III	2016	0	1965	36	0
1	JJJ	2018	0	1969	27	0
2	KKK	1599	0	1542	19	0
2	MMM	1401	0	1295	11	0
2	OOO	1593	0	1529	12	0
2	QQQ	1561	0	1458	16	0
2	TTT	1575	0	1501	9	0
2	VVV	1579	0	1521	6	0
2	XXX	1500	0	1418	13	0
2	YYY	1584	0	1528	21	0
2	bbb	1588	0	1515	8	0
2	ccc	1503	0	1438	14	0
3	LLL	1592	0	1506	34	0
3	NNN	1160	0	1073	26	0
3	PPP	1570	0	1453	21	0
3	RRR	1515	0	1436	31	0
3	SSS	1493	0	1418	22	0
3	UUU	1328	0	1288	16	0
3	WWW	1605	0	1526	24	0
3	ZZZ	1614	0	1567	16	0
3	aaa	1595	0	1530	28	0
3	ddd	1572	0	1510	29	0
4	AAA	22	0	0	0	0
4	BBB	31	0	0	0	0
4	CCC	27	0	0	0	0
4	DDD	23	0	0	0	0
4	EEE	29	0	0	1	0
4	FFF	22	0	0	0	0
4	GGG	35	0	0	1	0
4	HHH	34	0	0	0	0
4	III	31	0	0	0	0
4	JJJ	31	0	0	0	0
4	KKK	9	0	0	0	0
4	LLL	9	0	0	1	0
4	MMM	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	NNN	2	0	0	0	0
4	OOO	3	0	0	0	0
4	PPP	3	0	0	0	0
4	QQQ	6	0	0	0	0
4	RRR	4	0	0	0	0
4	SSS	3	0	0	0	0
4	TTT	2	0	0	0	0
4	UUU	2	0	0	0	0
4	VVV	3	0	0	0	0
4	WWW	1	0	0	0	0
4	XXX	1	0	0	0	0
4	YYY	1	0	0	0	0
4	ZZZ	1	0	0	0	0
4	bbb	1	0	0	0	0
4	ccc	4	0	0	0	0
4	ddd	2	0	0	0	0
All	All	51021	0	48728	594	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 6.

All (594) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:26:VAL:CG1	1:AAA:285:ARG:HH11	1.29	1.45
1:AAA:26:VAL:CG1	1:AAA:285:ARG:NH1	1.92	1.28
3:PPP:147:GLN:NE2	3:PPP:154:LEU:HD23	1.60	1.17
1:AAA:26:VAL:HG12	1:AAA:285:ARG:HH11	0.94	1.08
1:AAA:26:VAL:HG11	1:AAA:285:ARG:NH1	1.75	1.01
2:MMM:28:THR:HG23	2:MMM:31:SER:HB2	1.43	0.97
1:AAA:26:VAL:HG12	1:AAA:285:ARG:NH1	1.65	0.96
1:III:118:MET:HE1	1:JJJ:197:VAL:HG12	1.45	0.95
3:PPP:147:GLN:HE21	3:PPP:154:LEU:HD23	1.26	0.95
3:WWW:7:SER:OG	3:WWW:8:PRO:HD2	1.70	0.92
3:aaa:7:SER:HB3	3:aaa:8:PRO:HD2	1.51	0.90
1:FFF:118:MET:HE1	1:GGG:197:VAL:HG12	1.54	0.89
1:HHH:223:PRO:HB2	1:III:218:GLY:O	1.73	0.89
3:ddd:106:ILE:H	3:ddd:166:GLN:HE22	1.20	0.85
2:YYY:91:THR:HG22	2:YYY:121:VAL:H	1.44	0.83
1:AAA:27:LEU:O	1:AAA:285:ARG:HD2	1.78	0.82
3:WWW:7:SER:HB3	3:WWW:22:THR:H	1.43	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:197:VAL:CG1	1:EEE:118:MET:HE1	2.10	0.81
3:LLL:7:SER:OG	3:LLL:8:PRO:HD2	1.80	0.80
1:III:118:MET:HE1	1:JJJ:197:VAL:CG1	2.11	0.80
3:LLL:7:SER:HB3	3:LLL:22:THR:H	1.47	0.79
1:AAA:154:GLN:CD	1:AAA:181:MET:HE1	2.07	0.79
1:FFF:118:MET:HE1	1:GGG:197:VAL:CG1	2.12	0.78
3:UUU:154:LEU:HD12	3:UUU:154:LEU:O	1.87	0.75
3:NNN:7:SER:HB3	3:NNN:8:PRO:HD2	1.67	0.74
3:NNN:7:SER:HB2	3:NNN:22:THR:H	1.53	0.74
1:EEE:154:GLN:CD	1:EEE:181:MET:HE1	2.12	0.74
1:AAA:26:VAL:HG13	1:AAA:285:ARG:HH11	1.48	0.74
3:LLL:7:SER:HB3	3:LLL:22:THR:OG1	1.88	0.74
3:aaa:37:GLN:HB2	3:aaa:47:LEU:HD11	1.71	0.73
1:CCC:264:ASN:OD1	1:CCC:266:SER:OG	2.05	0.73
3:LLL:7:SER:CB	3:LLL:22:THR:H	2.01	0.72
3:aaa:7:SER:HB3	3:aaa:8:PRO:CD	2.19	0.72
2:YYY:170:THR:O	2:YYY:173:VAL:HG12	1.88	0.72
2:TTT:206:CYS:O	2:TTT:218:ASP:HA	1.90	0.71
3:UUU:150:VAL:HG12	3:UUU:150:VAL:O	1.89	0.71
2:QQQ:115:GLN:HA	3:RRR:43:ALA:HB2	1.72	0.71
3:RRR:8:PRO:O	3:RRR:102:THR:HG23	1.90	0.71
3:WWW:7:SER:CB	3:WWW:8:PRO:HD2	2.20	0.71
1:AAA:197:VAL:HG11	1:EEE:118:MET:HE1	1.70	0.71
3:ddd:7:SER:CB	3:ddd:8:PRO:CD	2.69	0.71
1:AAA:27:LEU:O	1:AAA:285:ARG:CD	2.39	0.70
3:SSS:7:SER:HB3	3:SSS:22:THR:OG1	1.90	0.70
3:ddd:7:SER:HB3	3:ddd:8:PRO:HD2	1.74	0.70
1:DDD:264:ASN:OD1	1:DDD:266:SER:HB3	1.91	0.69
3:PPP:7:SER:HB3	3:PPP:8:PRO:HD3	1.74	0.69
3:LLL:7:SER:CB	3:LLL:8:PRO:CD	2.70	0.69
3:WWW:119:PRO:HB3	3:WWW:209:PHE:CE2	2.27	0.69
3:PPP:147:GLN:HE22	3:PPP:154:LEU:HD23	1.52	0.69
1:HHH:154:GLN:CD	1:HHH:181:MET:HE1	2.18	0.69
1:BBB:118:MET:HE1	1:CCC:197:VAL:CG1	2.22	0.69
1:AAA:26:VAL:HG11	1:AAA:285:ARG:HH12	1.58	0.68
3:NNN:7:SER:HB3	3:NNN:8:PRO:CD	2.24	0.68
3:WWW:7:SER:CB	3:WWW:8:PRO:CD	2.72	0.68
3:aaa:7:SER:CB	3:aaa:8:PRO:CD	2.72	0.68
2:YYY:91:THR:HG22	2:YYY:121:VAL:N	2.08	0.67
3:NNN:7:SER:CB	3:NNN:8:PRO:CD	2.72	0.67
3:ddd:7:SER:OG	3:ddd:8:PRO:CD	2.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SSS:37:GLN:HB2	3:SSS:47:LEU:HD11	1.76	0.66
1:JJJ:112:ILE:HD11	1:JJJ:277:TYR:CB	2.25	0.66
3:ddd:106:ILE:N	3:ddd:166:GLN:HE22	1.91	0.65
3:ddd:7:SER:CB	3:ddd:8:PRO:HD2	2.27	0.65
3:LLL:7:SER:OG	3:LLL:8:PRO:CD	2.45	0.65
3:SSS:117:ILE:HD11	3:SSS:209:PHE:HE2	1.62	0.65
3:NNN:105:ASP:HB2	3:NNN:166:GLN:OE1	1.96	0.65
2:YYY:131:VAL:CG1	2:YYY:217:VAL:HG11	2.26	0.65
3:aaa:36:TYR:CE2	3:aaa:46:LEU:HD23	2.32	0.65
1:AAA:285:ARG:HG3	1:AAA:286:ARG:O	1.97	0.64
1:JJJ:120:VAL:HG22	1:JJJ:133:GLY:O	1.97	0.64
3:PPP:148:TRP:CD2	3:PPP:179:LEU:HD12	2.32	0.64
1:BBB:154:GLN:CD	1:BBB:181:MET:HE1	2.22	0.64
3:LLL:7:SER:HB2	3:LLL:8:PRO:HD3	1.80	0.64
1:BBB:118:MET:HE1	1:CCC:197:VAL:HG12	1.80	0.64
1:JJJ:218:GLY:O	1:JJJ:222:VAL:HG21	1.97	0.63
3:RRR:119:PRO:HB3	3:RRR:209:PHE:CE2	2.33	0.63
1:CCC:218:GLY:O	1:CCC:222:VAL:HG21	1.97	0.63
1:III:112:ILE:HD11	1:III:277:TYR:HB2	1.80	0.63
1:JJJ:154:GLN:CD	1:JJJ:181:MET:HE1	2.24	0.63
1:GGG:218:GLY:O	1:GGG:222:VAL:HG21	1.98	0.62
1:FFF:154:GLN:CD	1:FFF:181:MET:HE1	2.25	0.62
3:UUU:11:LEU:CD2	3:UUU:19:VAL:HG13	2.29	0.62
2:KKK:127:LYS:HE3	2:KKK:154:ASP:O	2.00	0.62
1:EEE:34:ASP:OD1	1:EEE:34:ASP:N	2.31	0.61
1:JJJ:84:ARG:HD3	1:JJJ:252:TYR:CZ	2.36	0.61
2:OOO:134:LEU:HB3	3:PPP:118:PHE:CD2	2.36	0.61
1:EEE:217:THR:HG22	1:EEE:222:VAL:HG11	1.81	0.61
3:SSS:108:ARG:NH1	3:SSS:109:THR:O	2.34	0.61
3:aaa:7:SER:CB	3:aaa:8:PRO:HD2	2.25	0.61
1:FFF:197:VAL:CG1	1:JJJ:118:MET:HE1	2.31	0.61
1:GGG:154:GLN:CD	1:GGG:181:MET:HE1	2.26	0.61
2:KKK:196:SER:OG	2:KKK:197:SER:N	2.25	0.61
3:PPP:141:PRO:O	3:PPP:198:HIS:HE1	1.84	0.61
2:YYY:131:VAL:HG11	2:YYY:217:VAL:HG11	1.83	0.60
1:JJJ:34:ASP:OD1	1:JJJ:34:ASP:N	2.35	0.60
2:KKK:211:LYS:HG2	2:KKK:212:PRO:HD3	1.83	0.60
1:BBB:112:ILE:HD11	1:BBB:277:TYR:HB2	1.83	0.60
3:RRR:7:SER:HB3	3:RRR:8:PRO:HD2	1.82	0.60
1:JJJ:112:ILE:HD11	1:JJJ:277:TYR:HB2	1.83	0.60
1:DDD:34:ASP:OD1	1:DDD:34:ASP:N	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NNN:115:VAL:HG23	3:NNN:136:LEU:HD13	1.83	0.59
2:TTT:91:THR:HG23	2:TTT:120:THR:HA	1.84	0.59
1:AAA:217:THR:HG22	1:AAA:222:VAL:HG11	1.84	0.59
2:MMM:28:THR:CG2	2:MMM:31:SER:HB2	2.26	0.59
3:RRR:37:GLN:HB2	3:RRR:47:LEU:HD11	1.84	0.59
3:SSS:6:GLN:NE2	3:SSS:86:TYR:O	2.36	0.59
3:ddd:7:SER:OG	3:ddd:8:PRO:HD3	2.03	0.59
1:HHH:112:ILE:HD11	1:HHH:277:TYR:HB2	1.84	0.59
3:NNN:7:SER:OG	3:NNN:8:PRO:HD3	2.03	0.58
3:RRR:7:SER:HB2	3:RRR:22:THR:OG1	2.04	0.58
1:AAA:216:LEU:HD13	1:EEE:114:VAL:O	2.03	0.58
1:BBB:157:LEU:HD23	1:BBB:199:CYS:HB3	1.84	0.58
1:III:112:ILE:HD11	1:III:277:TYR:CB	2.34	0.58
3:LLL:72:THR:HG23	4:LLL:309:HOH:O	2.03	0.58
3:RRR:105:ASP:OD1	3:RRR:173:TYR:OH	2.22	0.57
3:WWW:7:SER:HB2	3:WWW:8:PRO:CD	2.34	0.57
1:BBB:90:LEU:O	1:BBB:91:ASN:CB	2.52	0.57
2:YYY:91:THR:CG2	2:YYY:121:VAL:H	2.15	0.57
1:BBB:106:THR:OG1	1:BBB:281:GLN:HG3	2.05	0.57
3:ddd:105:ASP:OD1	3:ddd:173:TYR:OH	2.23	0.57
3:LLL:163:VAL:HG22	3:LLL:175:LEU:HD12	1.85	0.57
2:XXX:91:THR:HG23	2:XXX:120:THR:HA	1.86	0.57
3:SSS:22:THR:HG22	3:SSS:72:THR:HG22	1.86	0.57
1:GGG:103:GLU:OE1	1:GGG:285:ARG:HD3	2.05	0.56
3:ddd:7:SER:HB3	3:ddd:8:PRO:CD	2.34	0.56
1:AAA:129:ASP:OD2	3:PPP:27:GLN:NE2	2.38	0.56
1:HHH:157:LEU:HD21	1:HHH:171:PRO:HG2	1.87	0.56
1:AAA:118:MET:HE1	1:BBB:197:VAL:CG1	2.36	0.56
1:DDD:112:ILE:HD11	1:DDD:277:TYR:HB2	1.88	0.56
2:YYY:194:VAL:HG22	2:YYY:195:PRO:HD2	1.88	0.56
1:BBB:217:THR:HG22	1:BBB:222:VAL:HG11	1.87	0.56
1:EEE:24:VAL:HG13	1:EEE:287:VAL:HG13	1.87	0.56
3:NNN:37:GLN:HB2	3:NNN:47:LEU:HD11	1.88	0.56
1:GGG:281:GLN:HG3	4:GGG:309:HOH:O	2.04	0.56
1:III:154:GLN:CD	1:III:181:MET:HE1	2.31	0.55
1:AAA:120:VAL:HG22	1:AAA:133:GLY:O	2.07	0.55
1:GGG:112:ILE:HD11	1:GGG:277:TYR:N	2.22	0.55
2:KKK:153:LYS:HE2	2:KKK:181:GLN:OE1	2.06	0.55
3:aaa:21:ILE:HD12	3:aaa:102:THR:HB	1.89	0.55
1:DDD:123:ASN:O	1:DDD:264:ASN:HA	2.06	0.55
3:LLL:115:VAL:HG21	3:LLL:196:VAL:HG11	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SSS:7:SER:CB	3:SSS:8:PRO:HD3	2.37	0.55
3:aaa:6:GLN:HE21	3:aaa:21:ILE:HD11	1.72	0.55
2:QQQ:177:PRO:HG2	3:RRR:163:VAL:O	2.07	0.55
3:NNN:7:SER:CB	3:NNN:22:THR:H	2.19	0.55
1:DDD:218:GLY:O	1:DDD:222:VAL:HG21	2.05	0.55
1:AAA:26:VAL:HG13	1:AAA:285:ARG:HG2	1.89	0.54
3:aaa:155:GLN:OE1	3:aaa:158:ASN:ND2	2.40	0.54
3:RRR:54:LEU:HD21	3:RRR:58:VAL:O	2.07	0.54
3:RRR:154:LEU:C	3:RRR:154:LEU:HD13	2.32	0.54
1:DDD:154:GLN:CD	1:DDD:181:MET:HE1	2.32	0.54
1:JJJ:84:ARG:HD3	1:JJJ:252:TYR:OH	2.06	0.54
3:ddd:7:SER:CB	3:ddd:22:THR:H	2.20	0.54
3:LLL:7:SER:HB3	3:LLL:22:THR:N	2.18	0.54
1:DDD:157:LEU:O	1:DDD:179:GLN:HA	2.08	0.54
3:LLL:137:ASN:ND2	3:LLL:138:ASN:OD1	2.40	0.54
1:DDD:24:VAL:HG13	1:DDD:287:VAL:HG13	1.90	0.54
3:aaa:43:ALA:HB2	2:bbb:115:GLN:HA	1.90	0.54
1:AAA:197:VAL:HG12	1:EEE:118:MET:CE	2.38	0.54
1:AAA:197:VAL:HG12	1:EEE:118:MET:HE1	1.88	0.54
1:BBB:118:MET:CE	1:CCC:197:VAL:HG12	2.38	0.53
3:LLL:117:ILE:HD13	3:LLL:209:PHE:HD2	1.74	0.53
3:PPP:151:ASP:OD2	3:PPP:189:HIS:HB3	2.07	0.53
2:YYY:131:VAL:HG11	2:YYY:217:VAL:CG1	2.38	0.53
1:CCC:157:LEU:HD21	1:CCC:171:PRO:HG2	1.89	0.53
1:FFF:120:VAL:HG22	1:FFF:133:GLY:O	2.08	0.53
2:OOO:91:THR:HG23	2:OOO:120:THR:HA	1.91	0.53
1:FFF:181:MET:HE2	1:JJJ:42:PHE:CE2	2.43	0.53
3:aaa:6:GLN:HB2	3:aaa:100:PRO:HD2	1.90	0.53
3:LLL:7:SER:HB2	3:LLL:8:PRO:CD	2.38	0.53
3:PPP:163:VAL:HG12	3:PPP:164:THR:O	2.09	0.53
1:CCC:84:ARG:HG3	1:CCC:252:TYR:CZ	2.43	0.53
3:NNN:180:THR:O	3:NNN:181:LEU:HB2	2.08	0.53
3:UUU:11:LEU:HD21	3:UUU:19:VAL:HG13	1.91	0.53
2:YYY:27:PHE:CE2	2:YYY:98:ARG:HD3	2.43	0.53
3:ddd:7:SER:HB2	3:ddd:22:THR:O	2.08	0.53
1:III:33:VAL:O	1:III:34:ASP:HB2	2.08	0.53
3:UUU:163:VAL:HG12	3:UUU:164:THR:O	2.09	0.53
2:VVV:68:LEU:HD23	2:VVV:81:LEU:HD11	1.91	0.53
1:CCC:154:GLN:CD	1:CCC:181:MET:HE1	2.34	0.52
3:PPP:148:TRP:CG	3:PPP:179:LEU:HD12	2.44	0.52
3:SSS:7:SER:HB2	3:SSS:8:PRO:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:ddd:198:HIS:HB3	3:ddd:201:LEU:HD12	1.90	0.52
3:aaa:119:PRO:HB3	3:aaa:209:PHE:CE2	2.44	0.52
1:FFF:197:VAL:HG11	1:JJJ:118:MET:HE1	1.92	0.52
2:ccc:27:PHE:CE2	2:ccc:98:ARG:HD3	2.44	0.52
1:AAA:43:LEU:CD1	1:AAA:83:ALA:HB2	2.40	0.52
1:DDD:37:THR:HG22	1:DDD:102:TRP:CZ3	2.44	0.52
1:EEE:193:LYS:O	1:EEE:193:LYS:HG2	2.09	0.52
2:MMM:79:LEU:HD23	2:MMM:96:CYS:SG	2.49	0.52
2:YYY:71:SER:OG	2:YYY:80:TYR:HB2	2.09	0.52
1:FFF:25:GLU:O	1:FFF:287:VAL:HA	2.10	0.51
3:WWW:191:VAL:HG12	3:WWW:210:ASN:OD1	2.11	0.51
3:WWW:7:SER:HB3	3:WWW:22:THR:N	2.21	0.51
3:ddd:105:ASP:OD1	3:ddd:166:GLN:NE2	2.42	0.51
1:EEE:193:LYS:HG2	4:EEE:320:HOH:O	2.11	0.51
1:III:59:LYS:HE3	2:TTT:103:TYR:O	2.10	0.51
3:WWW:7:SER:OG	3:WWW:8:PRO:CD	2.51	0.51
2:ccc:207:ASN:ND2	2:ccc:218:ASP:OD1	2.39	0.51
3:LLL:37:GLN:HB2	3:LLL:47:LEU:HD11	1.92	0.51
3:UUU:105:ASP:OD1	3:UUU:173:TYR:OH	2.28	0.51
3:aaa:175:LEU:HD23	3:aaa:175:LEU:C	2.36	0.51
1:GGG:112:ILE:HD11	1:GGG:277:TYR:CB	2.41	0.51
1:III:120:VAL:HG22	1:III:133:GLY:O	2.10	0.51
2:YYY:111:ASP:HA	3:ZZZ:46:LEU:HD22	1.93	0.51
2:KKK:209:ASN:HD21	2:KKK:216:LYS:HE2	1.76	0.50
3:NNN:140:TYR:O	3:NNN:142:ARG:N	2.44	0.50
2:MMM:64:VAL:HB	2:MMM:68:LEU:HD22	1.93	0.50
3:ZZZ:24:ARG:HA	3:ZZZ:69:THR:O	2.11	0.50
3:aaa:18:ARG:HG3	3:aaa:76:SER:HA	1.91	0.50
1:GGG:41:CYS:SG	1:GGG:253:LEU:HD12	2.51	0.50
3:RRR:180:THR:O	3:RRR:181:LEU:HD23	2.11	0.50
1:DDD:171:PRO:HB3	1:DDD:185:HIS:CG	2.46	0.50
1:AAA:130:ASN:O	1:BBB:268:SER:HA	2.11	0.50
1:AAA:197:VAL:CG1	1:EEE:118:MET:CE	2.88	0.50
1:EEE:58:SER:HB3	1:EEE:271:TRP:HB2	1.94	0.50
1:III:118:MET:CE	1:JJJ:197:VAL:HG12	2.30	0.50
2:OOO:115:GLN:HG3	2:OOO:116:GLY:O	2.12	0.50
1:BBB:24:VAL:HG13	1:BBB:288:LYS:HG3	1.94	0.50
1:EEE:51:ASP:OD1	1:EEE:51:ASP:C	2.55	0.50
1:FFF:84:ARG:HD2	1:FFF:252:TYR:OH	2.12	0.50
1:HHH:118:MET:HE1	1:III:197:VAL:CG1	2.42	0.49
3:WWW:27:GLN:HG3	3:WWW:28:ARG:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:246:CYS:HB3	1:GGG:250:ASN:O	2.12	0.49
2:OOO:155:TYR:CE2	2:OOO:160:VAL:HG13	2.46	0.49
2:XXX:129:PRO:HD2	2:XXX:215:THR:HG21	1.94	0.49
2:OOO:170:THR:O	2:OOO:173:VAL:HG23	2.13	0.49
2:QQQ:83:LEU:HD12	2:QQQ:83:LEU:N	2.28	0.49
1:FFF:197:VAL:HG12	1:JJJ:118:MET:CE	2.43	0.49
3:ZZZ:117:ILE:HG22	3:ZZZ:207:LYS:HB3	1.94	0.49
1:EEE:218:GLY:O	1:EEE:222:VAL:HG21	2.12	0.49
2:XXX:170:THR:O	2:XXX:173:VAL:HG12	2.11	0.49
1:DDD:186:LYS:NZ	1:DDD:203:ASP:OD2	2.33	0.49
2:KKK:12:VAL:O	2:KKK:121:VAL:HA	2.12	0.49
2:KKK:194:VAL:HG11	2:KKK:204:TYR:OH	2.12	0.49
3:RRR:146:VAL:HG23	3:RRR:146:VAL:O	2.12	0.49
3:UUU:201:LEU:HD13	3:UUU:205:VAL:CG2	2.43	0.49
2:XXX:179:VAL:O	2:XXX:186:TYR:HA	2.12	0.49
2:ccc:129:PRO:HB3	2:ccc:155:TYR:HB3	1.95	0.49
1:FFF:156:VAL:HG21	1:JJJ:112:ILE:HG22	1.94	0.49
2:ccc:181:GLN:HG2	2:ccc:185:LEU:O	2.11	0.49
1:III:154:GLN:OE1	1:III:181:MET:HE1	2.13	0.49
2:MMM:28:THR:HG23	2:MMM:28:THR:O	2.13	0.49
1:AAA:154:GLN:NE2	1:AAA:181:MET:HE1	2.28	0.49
1:CCC:180:VAL:O	1:CCC:181:MET:HB2	2.12	0.49
3:SSS:7:SER:CB	3:SSS:8:PRO:CD	2.90	0.49
1:III:24:VAL:HG13	1:III:287:VAL:HG13	1.95	0.48
3:ZZZ:61:ARG:CZ	3:ZZZ:79:GLN:HG3	2.43	0.48
2:bbb:64:VAL:HB	2:bbb:68:LEU:HG	1.94	0.48
2:bbb:172:GLY:O	2:bbb:192:VAL:HA	2.12	0.48
1:BBB:118:MET:HE1	1:CCC:197:VAL:HG11	1.96	0.48
1:CCC:264:ASN:ND2	1:CCC:268:SER:OG	2.29	0.48
2:XXX:12:VAL:HG21	2:XXX:18:LEU:HD22	1.95	0.48
1:JJJ:155:GLY:HA2	1:JJJ:199:CYS:O	2.13	0.48
2:KKK:145:THR:HG23	2:KKK:145:THR:O	2.13	0.48
3:PPP:150:VAL:HG12	3:PPP:192:TYR:CD1	2.49	0.48
3:UUU:142:ARG:NH1	3:UUU:163:VAL:HG21	2.29	0.48
1:EEE:84:ARG:HD3	1:EEE:252:TYR:OH	2.14	0.48
3:LLL:21:ILE:HD11	3:LLL:73:LEU:HD23	1.96	0.48
2:MMM:164:TRP:CZ3	2:MMM:206:CYS:HB3	2.48	0.48
2:OOO:114:GLY:O	3:PPP:43:ALA:HB2	2.14	0.48
2:TTT:161:THR:O	2:TTT:208:VAL:HA	2.13	0.48
3:ZZZ:21:ILE:HD11	3:ZZZ:73:LEU:HD23	1.96	0.48
1:FFF:34:ASP:OD1	1:FFF:34:ASP:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:RRR:132:VAL:HG12	3:RRR:148:TRP:CH2	2.48	0.48
3:WWW:19:VAL:HG21	3:WWW:78:LEU:HD22	1.96	0.48
3:ZZZ:182:SER:OG	3:ZZZ:185:ASP:OD1	2.32	0.48
3:aaa:7:SER:CB	3:aaa:22:THR:H	2.27	0.48
2:KKK:91:THR:HG23	2:KKK:120:THR:HA	1.96	0.47
1:BBB:149:GLU:HG2	1:BBB:209:ASN:HD22	1.78	0.47
3:PPP:129:THR:HA	3:PPP:182:SER:HA	1.96	0.47
1:AAA:157:LEU:O	1:AAA:179:GLN:HA	2.15	0.47
3:RRR:151:ASP:HA	3:RRR:191:VAL:HG13	1.95	0.47
3:ddd:147:GLN:CG	3:ddd:154:LEU:HD21	2.45	0.47
2:KKK:111:ASP:HA	3:LLL:46:LEU:HD22	1.96	0.47
2:QQQ:173:VAL:HG22	2:QQQ:192:VAL:HG22	1.96	0.47
3:WWW:203:SER:OG	3:WWW:204:PRO:HD2	2.13	0.47
2:YYY:88:THR:O	2:YYY:91:THR:HG23	2.14	0.47
1:BBB:171:PRO:HB3	1:BBB:185:HIS:CG	2.49	0.47
1:EEE:68:GLU:HG3	1:EEE:161:ARG:NH1	2.30	0.47
1:III:123:ASN:O	1:III:264:ASN:HA	2.14	0.47
1:AAA:108:LYS:NZ	1:AAA:230:ASN:O	2.46	0.47
1:AAA:118:MET:HE1	1:BBB:197:VAL:HG11	1.97	0.47
1:EEE:109:THR:HA	1:EEE:277:TYR:O	2.14	0.47
3:SSS:11:LEU:HD21	3:SSS:19:VAL:HG13	1.97	0.47
2:TTT:194:VAL:HG11	2:TTT:204:TYR:CZ	2.49	0.47
2:ccc:68:LEU:HD22	2:ccc:83:LEU:HA	1.96	0.47
1:AAA:26:VAL:HG13	1:AAA:285:ARG:NH1	2.14	0.47
3:RRR:107:LYS:HA	3:RRR:140:TYR:OH	2.15	0.47
2:XXX:205:ILE:CD1	2:XXX:207:ASN:HD21	2.28	0.47
1:EEE:37:THR:HG22	1:EEE:102:TRP:CZ3	2.49	0.47
1:EEE:154:GLN:OE1	1:EEE:181:MET:HE1	2.14	0.47
1:HHH:99:ILE:HG23	1:HHH:287:VAL:O	2.15	0.47
3:SSS:197:THR:HG22	3:SSS:204:PRO:HB3	1.97	0.47
2:YYY:211:LYS:HB2	2:YYY:212:PRO:HD3	1.95	0.47
1:BBB:105:VAL:HG12	1:BBB:106:THR:HG23	1.97	0.47
1:CCC:118:MET:HE1	1:DDD:197:VAL:CG1	2.45	0.46
2:QQQ:147:ALA:HB3	3:RRR:116:PHE:CD2	2.50	0.46
1:GGG:217:THR:HG22	1:GGG:222:VAL:HG11	1.97	0.46
1:JJJ:100:LEU:HD23	1:JJJ:286:ARG:HA	1.97	0.46
2:MMM:114:GLY:O	3:NNN:43:ALA:CB	2.64	0.46
2:OOO:68:LEU:HG	2:OOO:83:LEU:HD23	1.96	0.46
1:BBB:112:ILE:HD11	1:BBB:277:TYR:CB	2.45	0.46
1:III:109:THR:HA	1:III:277:TYR:O	2.15	0.46
3:LLL:7:SER:CB	3:LLL:8:PRO:HD3	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:UUU:133:VAL:HG21	2:XXX:134:LEU:HD11	1.98	0.46
3:WWW:89:GLN:HB2	3:WWW:98:PHE:CD1	2.51	0.46
3:ddd:135:LEU:CD1	3:ddd:137:ASN:HB2	2.45	0.46
1:AAA:41:CYS:SG	1:AAA:253:LEU:HD12	2.55	0.46
1:FFF:194:ALA:O	1:FFF:196:PRO:HD3	2.14	0.46
3:LLL:21:ILE:CG2	3:LLL:102:THR:HG21	2.45	0.46
2:MMM:108:TYR:HB2	3:NNN:96:PRO:HG3	1.98	0.46
3:LLL:150:VAL:HG23	3:LLL:155:GLN:HG3	1.96	0.46
3:ddd:7:SER:OG	3:ddd:8:PRO:HD2	2.15	0.46
1:AAA:120:VAL:HG11	1:BBB:261:MET:HE1	1.98	0.46
1:FFF:109:THR:HA	1:FFF:277:TYR:O	2.16	0.46
1:AAA:118:MET:HE1	1:BBB:197:VAL:HG12	1.97	0.46
1:DDD:112:ILE:HD11	1:DDD:277:TYR:CB	2.45	0.46
1:FFF:84:ARG:HG3	1:FFF:252:TYR:CZ	2.51	0.46
1:GGG:112:ILE:HD11	1:GGG:277:TYR:HB2	1.97	0.46
3:RRR:78:LEU:CD1	3:RRR:82:ASP:HB2	2.46	0.46
2:ccc:67:ARG:C	2:ccc:68:LEU:HD23	2.40	0.46
2:ccc:173:VAL:HG12	2:ccc:192:VAL:HB	1.98	0.46
1:CCC:42:PHE:CD1	1:DDD:181:MET:HG2	2.51	0.46
3:LLL:186:TYR:O	3:LLL:192:TYR:OH	2.33	0.45
3:PPP:155:GLN:OE1	3:PPP:158:ASN:ND2	2.46	0.45
3:aaa:201:LEU:HD13	3:aaa:205:VAL:HG23	1.98	0.45
3:PPP:146:VAL:HG12	3:PPP:161:GLU:OE2	2.17	0.45
3:WWW:7:SER:CB	3:WWW:22:THR:H	2.22	0.45
3:ddd:7:SER:HA	3:ddd:22:THR:OG1	2.17	0.45
1:AAA:123:ASN:O	1:AAA:264:ASN:HA	2.16	0.45
1:CCC:43:LEU:HD11	1:CCC:83:ALA:HB2	1.98	0.45
1:CCC:171:PRO:HB3	1:CCC:185:HIS:CG	2.51	0.45
2:KKK:131:VAL:HG21	2:KKK:208:VAL:HG21	1.98	0.45
3:RRR:24:ARG:HA	3:RRR:69:THR:O	2.16	0.45
3:RRR:147:GLN:OE1	3:RRR:154:LEU:HD21	2.15	0.45
3:WWW:7:SER:HB2	3:WWW:8:PRO:HD2	1.96	0.45
1:JJJ:152:GLU:HB3	1:JJJ:206:ARG:CZ	2.47	0.45
3:ddd:37:GLN:HB2	3:ddd:47:LEU:HD11	1.97	0.45
1:CCC:154:GLN:OE1	1:CCC:181:MET:HE1	2.15	0.45
1:GGG:66:THR:OG1	1:GGG:68:GLU:HG2	2.17	0.45
3:UUU:195:GLU:HA	3:UUU:205:VAL:O	2.16	0.45
1:BBB:41:CYS:SG	1:BBB:253:LEU:HD12	2.57	0.45
1:FFF:119:ASN:OD1	1:FFF:119:ASN:C	2.60	0.45
2:KKK:88:THR:HA	2:KKK:121:VAL:HB	1.99	0.45
2:KKK:211:LYS:N	2:KKK:212:PRO:CD	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QQQ:111:ASP:HA	3:RRR:46:LEU:HD22	1.98	0.45
2:YYY:193:THR:HG21	3:ZZZ:137:ASN:HD22	1.81	0.45
3:ZZZ:33:LEU:HD13	3:ZZZ:34:ASN:N	2.31	0.45
2:ccc:211:LYS:N	2:ccc:212:PRO:CD	2.80	0.45
1:CCC:261:MET:HA	1:CCC:270:GLN:O	2.17	0.45
1:EEE:145:SER:OG	1:EEE:254:SER:HB2	2.17	0.45
1:GGG:235:VAL:HG12	1:GGG:237:LEU:H	1.82	0.45
3:NNN:7:SER:HB2	3:NNN:22:THR:N	2.27	0.45
3:NNN:113:PRO:HB3	3:NNN:139:PHE:CD2	2.52	0.45
2:VVV:111:ASP:HA	3:WWW:46:LEU:HD22	1.99	0.45
2:XXX:155:TYR:CE2	2:XXX:160:VAL:HG23	2.52	0.45
1:CCC:105:VAL:HG21	1:CCC:283:ARG:HD3	1.98	0.45
3:NNN:166:GLN:HG3	3:NNN:173:TYR:CZ	2.51	0.45
3:WWW:163:VAL:HG12	3:WWW:164:THR:O	2.17	0.45
1:III:194:ALA:O	1:III:196:PRO:HD3	2.15	0.45
3:LLL:19:VAL:HG21	3:LLL:78:LEU:HD13	1.98	0.45
3:PPP:198:HIS:CD2	3:PPP:200:GLY:H	2.35	0.45
3:RRR:21:ILE:HD12	3:RRR:73:LEU:HD23	1.98	0.45
1:EEE:114:VAL:HG12	1:EEE:226:LEU:HD13	1.98	0.45
1:III:81:SER:HA	1:III:192:ASN:OD1	2.16	0.45
2:KKK:210:HIS:CE1	2:KKK:213:SER:HB2	2.52	0.45
2:QQQ:48:VAL:HG13	2:QQQ:64:VAL:HG21	1.98	0.45
1:AAA:25:GLU:O	1:AAA:287:VAL:HA	2.17	0.44
1:III:64:SER:HB3	1:III:70:ASP:HA	1.99	0.44
1:JJJ:128:HIS:HD2	1:JJJ:129:ASP:O	2.00	0.44
3:NNN:122:ASP:C	3:NNN:123:GLU:OE1	2.60	0.44
3:ZZZ:112:ALA:HB1	3:ZZZ:201:LEU:HD21	2.00	0.44
3:aaa:120:PRO:HD3	3:aaa:132:VAL:HG22	1.98	0.44
1:FFF:64:SER:HB3	1:FFF:70:ASP:HA	1.98	0.44
1:GGG:61:ILE:HG12	1:GGG:269:GLN:O	2.18	0.44
3:LLL:195:GLU:HG3	3:LLL:206:THR:HG22	1.98	0.44
3:SSS:47:LEU:HA	3:SSS:58:VAL:HG21	1.99	0.44
1:BBB:154:GLN:OE1	1:BBB:181:MET:HE1	2.15	0.44
3:NNN:11:LEU:O	3:NNN:104:VAL:HA	2.17	0.44
3:UUU:7:SER:HB3	3:UUU:8:PRO:HD3	1.99	0.44
3:ZZZ:7:SER:HB3	3:ZZZ:8:PRO:HD3	1.98	0.44
1:HHH:171:PRO:HB3	1:HHH:185:HIS:ND1	2.33	0.44
3:NNN:135:LEU:C	3:NNN:135:LEU:HD12	2.43	0.44
2:TTT:161:THR:OG1	2:TTT:209:ASN:HB3	2.17	0.44
2:YYY:180:LEU:HD13	2:YYY:186:TYR:CZ	2.52	0.44
3:aaa:7:SER:HB2	3:aaa:22:THR:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:25:GLU:O	1:HHH:287:VAL:HA	2.18	0.44
1:III:106:THR:OG1	1:III:281:GLN:OE1	2.34	0.44
2:OOO:12:VAL:HG21	2:OOO:18:LEU:HD22	2.00	0.44
2:QQQ:169:LEU:HD21	2:QQQ:192:VAL:HG11	2.00	0.44
3:WWW:135:LEU:C	3:WWW:136:LEU:HD23	2.42	0.44
1:FFF:197:VAL:HG12	1:JJJ:118:MET:HE1	1.98	0.44
3:UUU:37:GLN:HG3	3:UUU:86:TYR:CE2	2.52	0.44
2:YYY:134:LEU:HB3	3:ZZZ:118:PHE:CD2	2.52	0.44
3:ZZZ:37:GLN:O	3:ZZZ:44:PRO:HA	2.18	0.44
3:aaa:142:ARG:O	3:aaa:142:ARG:HG2	2.17	0.44
2:bbb:73:ASP:OD1	2:bbb:75:SER:OG	2.25	0.44
2:ccc:53:TYR:CG	2:ccc:54:ASP:N	2.86	0.44
3:ddd:135:LEU:HD11	3:ddd:137:ASN:HB2	1.99	0.44
1:DDD:35:SER:HA	1:DDD:284:LYS:HE3	2.00	0.44
1:HHH:171:PRO:HB3	1:HHH:185:HIS:CG	2.53	0.44
1:AAA:43:LEU:HD11	1:AAA:83:ALA:HB2	2.00	0.44
1:JJJ:41:CYS:SG	1:JJJ:253:LEU:HD12	2.58	0.44
3:LLL:22:THR:HG22	3:LLL:72:THR:HG22	2.00	0.44
2:OOO:12:VAL:CG2	2:OOO:18:LEU:HD22	2.48	0.44
1:FFF:122:SER:HB2	1:GGG:70:ASP:OD2	2.18	0.44
3:LLL:180:THR:O	3:LLL:181:LEU:HD23	2.17	0.44
1:DDD:262:PHE:CD1	1:EEE:158:PHE:HZ	2.37	0.43
1:FFF:80:TYR:CE1	1:FFF:197:VAL:HA	2.52	0.43
1:FFF:123:ASN:O	1:FFF:264:ASN:HA	2.18	0.43
1:GGG:38:GLU:OE1	1:GGG:281:GLN:NE2	2.51	0.43
3:NNN:115:VAL:O	3:NNN:115:VAL:HG13	2.18	0.43
3:RRR:136:LEU:HD21	3:RRR:196:VAL:HG13	2.00	0.43
3:RRR:162:SER:O	3:RRR:175:LEU:HD22	2.18	0.43
1:EEE:157:LEU:HD21	1:EEE:171:PRO:HG2	2.00	0.43
2:KKK:53:TYR:CG	2:KKK:54:ASP:N	2.86	0.43
2:OOO:84:ASN:O	2:OOO:85:SER:C	2.60	0.43
1:FFF:139:THR:O	1:FFF:260:GLY:HA2	2.19	0.43
1:III:211:ARG:HD3	1:III:211:ARG:N	2.33	0.43
3:LLL:34:ASN:O	3:LLL:88:CYS:HA	2.17	0.43
1:AAA:70:ASP:OD2	1:AAA:162:THR:OG1	2.29	0.43
1:III:129:ASP:O	1:III:130:ASN:HB2	2.18	0.43
3:PPP:186:TYR:CD1	3:PPP:192:TYR:CE2	3.06	0.43
3:SSS:117:ILE:CD1	3:SSS:209:PHE:HE2	2.30	0.43
3:aaa:149:LYS:HE3	3:aaa:195:GLU:OE1	2.19	0.43
1:HHH:154:GLN:OE1	1:HHH:181:MET:HE1	2.17	0.43
1:III:261:MET:HE3	1:III:271:TRP:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:24:ARG:HA	3:LLL:69:THR:O	2.18	0.43
2:QQQ:51:ILE:HG12	2:QQQ:55:GLY:HA2	1.99	0.43
2:VVV:53:TYR:CG	2:VVV:54:ASP:N	2.86	0.43
2:ccc:211:LYS:N	2:ccc:212:PRO:HD2	2.34	0.43
1:FFF:122:SER:HB2	1:GGG:70:ASP:CG	2.44	0.43
1:JJJ:163:LYS:HA	1:JJJ:163:LYS:HD3	1.79	0.43
2:KKK:194:VAL:CG1	2:KKK:204:TYR:OH	2.67	0.43
3:RRR:113:PRO:HB3	3:RRR:139:PHE:HB3	2.00	0.43
2:VVV:12:VAL:O	2:VVV:121:VAL:HA	2.18	0.43
3:ddd:186:TYR:CE1	3:ddd:192:TYR:CE2	3.06	0.43
1:AAA:120:VAL:CG2	1:AAA:133:GLY:O	2.66	0.43
1:AAA:212:TYR:CE2	1:EEE:230:ASN:HB3	2.53	0.43
1:GGG:103:GLU:O	1:GGG:282:LEU:HA	2.18	0.43
1:III:57:PHE:CE2	1:III:272:ARG:HD3	2.54	0.43
3:SSS:7:SER:OG	3:SSS:8:PRO:CD	2.67	0.43
3:SSS:145:LYS:HD3	3:SSS:145:LYS:HA	1.78	0.43
1:EEE:43:LEU:HD11	1:EEE:83:ALA:HB2	1.99	0.43
1:FFF:118:MET:CE	1:GGG:197:VAL:HG12	2.36	0.43
1:III:182:ASN:HB3	1:III:185:HIS:CD2	2.53	0.43
3:SSS:3:GLN:N	3:SSS:26:SER:OG	2.43	0.43
3:UUU:162:SER:OG	2:XXX:177:PRO:O	2.29	0.43
3:ddd:29:ILE:O	3:ddd:30:SER:C	2.62	0.43
1:GGG:64:SER:HB2	1:GGG:69:SER:OG	2.18	0.43
1:HHH:182:ASN:HB3	1:HHH:185:HIS:CD2	2.54	0.43
3:LLL:113:PRO:HB3	3:LLL:139:PHE:HB3	2.00	0.43
3:UUU:154:LEU:HD12	3:UUU:154:LEU:C	2.43	0.43
2:YYY:177:PRO:O	3:ZZZ:162:SER:OG	2.34	0.43
3:aaa:21:ILE:HG23	3:aaa:73:LEU:HB3	2.01	0.43
1:HHH:109:THR:HA	1:HHH:277:TYR:O	2.19	0.42
1:BBB:89:ASN:HA	1:BBB:249:ASP:OD2	2.20	0.42
1:DDD:154:GLN:OE1	1:DDD:181:MET:HE1	2.18	0.42
1:HHH:32:GLY:O	1:HHH:35:SER:HB3	2.19	0.42
1:HHH:89:ASN:HA	1:HHH:249:ASP:OD2	2.20	0.42
3:LLL:136:LEU:HD21	3:LLL:196:VAL:CG2	2.49	0.42
2:YYY:164:TRP:CZ3	2:YYY:206:CYS:HB3	2.54	0.42
1:GGG:109:THR:HA	1:GGG:277:TYR:O	2.19	0.42
2:TTT:73:ASP:OD2	2:TTT:75:SER:OG	2.38	0.42
3:WWW:136:LEU:HD23	3:WWW:136:LEU:N	2.34	0.42
3:aaa:186:TYR:O	3:aaa:192:TYR:OH	2.34	0.42
2:ccc:73:ASP:OD1	2:ccc:75:SER:OG	2.21	0.42
1:AAA:218:GLY:O	1:AAA:222:VAL:HG21	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NNN:140:TYR:H	3:NNN:141:PRO:HD2	1.83	0.42
2:QQQ:210:HIS:ND1	2:QQQ:213:SER:HB3	2.34	0.42
1:AAA:54:LEU:HA	1:BBB:179:GLN:HE22	1.84	0.42
1:DDD:35:SER:O	1:DDD:283:ARG:HA	2.20	0.42
2:KKK:162:VAL:HA	2:KKK:207:ASN:O	2.20	0.42
3:WWW:151:ASP:OD1	3:WWW:191:VAL:HG22	2.18	0.42
2:ccc:181:GLN:HB3	3:ddd:160:GLN:HE22	1.84	0.42
1:EEE:43:LEU:HD12	1:EEE:43:LEU:HA	1.90	0.42
2:QQQ:115:GLN:H	2:QQQ:115:GLN:HG3	1.73	0.42
3:SSS:21:ILE:HD12	3:SSS:73:LEU:HD23	2.00	0.42
2:TTT:160:VAL:HG22	2:TTT:210:HIS:HB2	2.01	0.42
3:ZZZ:48:ILE:CD1	3:ZZZ:54:LEU:HD12	2.49	0.42
1:GGG:154:GLN:OE1	1:GGG:181:MET:HE1	2.18	0.42
3:LLL:194:CYS:O	3:LLL:206:THR:HA	2.19	0.42
3:ddd:54:LEU:HD21	3:ddd:58:VAL:O	2.19	0.42
3:ddd:124:GLN:HE21	3:ddd:129:THR:HG23	1.84	0.42
1:III:160:TYR:CD1	1:III:176:VAL:HA	2.55	0.42
2:QQQ:162:VAL:HG12	2:QQQ:208:VAL:HG12	2.02	0.42
3:SSS:7:SER:CB	3:SSS:22:THR:OG1	2.63	0.42
3:SSS:24:ARG:HA	3:SSS:69:THR:O	2.19	0.42
3:aaa:21:ILE:CD1	3:aaa:102:THR:HB	2.49	0.42
3:aaa:160:GLN:NE2	2:bbb:180:LEU:O	2.53	0.42
1:CCC:145:SER:OG	1:CCC:254:SER:HB2	2.20	0.42
1:DDD:43:LEU:HD12	1:DDD:43:LEU:HA	1.80	0.42
1:DDD:151:LEU:HD12	1:DDD:207:ASN:OD1	2.19	0.42
1:EEE:196:PRO:HB2	1:EEE:199:CYS:SG	2.60	0.42
1:HHH:277:TYR:CD2	1:III:204:PRO:HB2	2.54	0.42
1:III:142:HIS:O	1:III:214:GLY:HA2	2.20	0.42
2:QQQ:134:LEU:HB3	3:RRR:118:PHE:CD1	2.54	0.42
3:SSS:117:ILE:CD1	3:SSS:209:PHE:CE2	3.03	0.42
3:UUU:42:LYS:HA	2:XXX:115:GLN:HE22	1.84	0.42
1:FFF:230:ASN:HB3	1:GGG:212:TYR:CE2	2.55	0.41
1:III:29:VAL:HG11	1:III:283:ARG:HD2	2.00	0.41
1:AAA:43:LEU:HA	1:AAA:43:LEU:HD12	1.76	0.41
1:DDD:103:GLU:HA	1:DDD:244:PRO:O	2.20	0.41
2:XXX:205:ILE:HD12	2:XXX:207:ASN:HD21	1.83	0.41
2:bbb:181:GLN:HG3	2:bbb:185:LEU:O	2.20	0.41
2:ccc:67:ARG:O	2:ccc:68:LEU:HD23	2.20	0.41
3:ddd:136:LEU:HD21	3:ddd:146:VAL:CG2	2.50	0.41
1:CCC:157:LEU:O	1:CCC:179:GLN:HA	2.19	0.41
1:FFF:106:THR:OG1	1:FFF:281:GLN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:171:PRO:HB3	1:JJJ:185:HIS:CG	2.55	0.41
2:OOO:36:TRP:CE2	2:OOO:81:LEU:HB2	2.56	0.41
3:RRR:136:LEU:HD21	3:RRR:196:VAL:CG1	2.50	0.41
3:RRR:151:ASP:HA	3:RRR:191:VAL:CG1	2.51	0.41
2:TTT:12:VAL:HG11	2:TTT:18:LEU:HD22	2.03	0.41
3:WWW:37:GLN:HB2	3:WWW:47:LEU:HD11	2.02	0.41
2:YYY:131:VAL:HG12	2:YYY:217:VAL:HG11	2.01	0.41
1:BBB:180:VAL:HG23	1:BBB:181:MET:N	2.36	0.41
1:BBB:211:ARG:HD3	1:BBB:211:ARG:N	2.36	0.41
1:CCC:160:TYR:CD2	1:CCC:176:VAL:HA	2.56	0.41
1:III:26:VAL:HG13	1:III:285:ARG:HD3	2.02	0.41
1:III:43:LEU:HD11	1:III:83:ALA:HB2	2.03	0.41
3:LLL:60:SER:HB2	2:QQQ:89:GLU:OE2	2.21	0.41
3:NNN:7:SER:HB2	3:NNN:22:THR:O	2.20	0.41
3:RRR:7:SER:CB	3:RRR:8:PRO:HD2	2.48	0.41
3:RRR:78:LEU:HD12	3:RRR:82:ASP:HB2	2.02	0.41
3:WWW:198:HIS:HB3	3:WWW:201:LEU:CD1	2.50	0.41
2:KKK:68:LEU:HD23	2:KKK:81:LEU:HD11	2.03	0.41
3:NNN:181:LEU:HD12	3:NNN:181:LEU:HA	1.89	0.41
1:AAA:213:PHE:CZ	1:EEE:231:THR:HG21	2.55	0.41
1:FFF:43:LEU:HD12	1:FFF:43:LEU:HA	1.91	0.41
1:JJJ:123:ASN:O	1:JJJ:264:ASN:HA	2.19	0.41
2:KKK:210:HIS:CD2	2:KKK:212:PRO:HD2	2.56	0.41
3:SSS:117:ILE:HD11	3:SSS:209:PHE:CE2	2.49	0.41
2:VVV:201:THR:O	2:VVV:201:THR:OG1	2.33	0.41
1:BBB:37:THR:HG22	1:BBB:282:LEU:HB2	2.03	0.41
1:BBB:141:PHE:HD2	1:BBB:256:VAL:HG11	1.85	0.41
1:CCC:130:ASN:O	1:DDD:268:SER:HA	2.20	0.41
1:FFF:43:LEU:HD11	1:FFF:83:ALA:HB2	2.02	0.41
1:HHH:118:MET:HE1	1:III:197:VAL:HG11	2.03	0.41
1:III:119:ASN:OD1	1:III:119:ASN:C	2.64	0.41
3:aaa:210:ASN:O	3:aaa:211:ARG:C	2.64	0.41
1:HHH:122:SER:HB2	1:III:70:ASP:CG	2.46	0.41
2:QQQ:194:VAL:HG11	2:QQQ:204:TYR:CZ	2.55	0.41
3:ZZZ:163:VAL:CG2	3:ZZZ:175:LEU:HD12	2.51	0.41
3:aaa:151:ASP:O	3:aaa:152:ASN:HB2	2.21	0.41
3:ddd:4:MET:HE1	3:ddd:25:ALA:HB2	2.03	0.41
3:ddd:108:ARG:HH12	3:ddd:111:ALA:HB3	1.86	0.41
1:EEE:211:ARG:N	1:EEE:211:ARG:HD3	2.35	0.41
1:GGG:192:ASN:O	1:GGG:193:LYS:HB2	2.20	0.41
1:HHH:157:LEU:O	1:HHH:179:GLN:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:223:PRO:HA	1:HHH:224:PRO:HD3	1.95	0.41
1:III:217:THR:HG22	1:III:222:VAL:HG11	2.03	0.41
2:MMM:35:HIS:CE1	2:MMM:50:VAL:CG2	3.04	0.41
3:NNN:136:LEU:HD23	3:NNN:175:LEU:HB3	2.01	0.41
3:RRR:146:VAL:O	3:RRR:146:VAL:CG2	2.69	0.41
2:YYY:133:PRO:HD2	3:ZZZ:121:SER:HB3	2.02	0.41
2:bbb:102:GLY:O	2:bbb:103:TYR:C	2.63	0.41
1:BBB:153:LEU:HD11	1:BBB:189:LEU:HB2	2.02	0.41
1:BBB:157:LEU:CD2	1:BBB:199:CYS:HB3	2.48	0.41
1:FFF:29:VAL:HG12	1:FFF:30:LYS:O	2.21	0.41
1:FFF:268:SER:HA	1:JJJ:130:ASN:O	2.21	0.41
1:III:112:ILE:HD11	1:III:277:TYR:N	2.36	0.41
3:ddd:108:ARG:HD2	3:ddd:171:SER:HB2	2.03	0.41
1:GGG:160:TYR:CE1	1:GGG:161:ARG:HG3	2.56	0.40
1:JJJ:30:LYS:HD2	1:JJJ:100:LEU:HD11	2.03	0.40
3:LLL:136:LEU:HD21	3:LLL:196:VAL:HG21	2.03	0.40
3:PPP:105:ASP:C	3:PPP:105:ASP:OD1	2.64	0.40
2:QQQ:173:VAL:HG23	2:QQQ:192:VAL:HG13	2.02	0.40
3:RRR:190:LYS:O	3:RRR:210:ASN:HA	2.21	0.40
2:bbb:48:VAL:CG1	2:bbb:68:LEU:HD12	2.51	0.40
2:ccc:34:MET:HB3	2:ccc:79:LEU:HD22	2.03	0.40
1:BBB:99:ILE:O	1:BBB:286:ARG:HA	2.22	0.40
1:BBB:183:THR:O	1:BBB:184:GLU:C	2.64	0.40
3:UUU:113:PRO:HD2	3:UUU:201:LEU:HD12	2.02	0.40
3:WWW:134:CYS:HB2	3:WWW:148:TRP:CZ2	2.56	0.40
3:aaa:185:ASP:HA	3:aaa:188:LYS:HG3	2.03	0.40
1:FFF:105:VAL:HG12	1:FFF:106:THR:HG23	2.02	0.40
3:LLL:2:ILE:HD13	3:LLL:29:ILE:CG2	2.51	0.40
3:LLL:124:GLN:O	3:LLL:127:SER:OG	2.37	0.40
2:XXX:50:VAL:CG1	2:XXX:59:LEU:HB2	2.52	0.40
2:XXX:205:ILE:HA	2:XXX:219:LYS:O	2.21	0.40
1:DDD:217:THR:HG22	1:DDD:222:VAL:HG11	2.03	0.40
1:III:40:GLU:O	1:III:41:CYS:HB3	2.21	0.40
2:MMM:114:GLY:O	3:NNN:43:ALA:HB2	2.21	0.40
3:PPP:186:TYR:CD1	3:PPP:192:TYR:HE2	2.39	0.40
3:SSS:54:LEU:HD11	3:SSS:58:VAL:HG12	2.04	0.40
2:YYY:194:VAL:CG2	2:YYY:195:PRO:HD2	2.50	0.40
3:aaa:107:LYS:HA	3:aaa:140:TYR:OH	2.21	0.40
3:ddd:24:ARG:HA	3:ddd:69:THR:O	2.22	0.40
2:MMM:107:THR:HA	3:NNN:91:SER:O	2.21	0.40
2:OOO:175:THR:HG23	2:OOO:190:SER:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PPP:83:PHE:CE1	3:PPP:106:ILE:HA	2.57	0.40
2:VVV:203:THR:HG22	2:VVV:220:LYS:HE3	2.04	0.40
3:WWW:12:SER:HA	3:WWW:105:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	255/272 (94%)	240 (94%)	15 (6%)	0	100	100
1	BBB	254/272 (93%)	242 (95%)	12 (5%)	0	100	100
1	CCC	254/272 (93%)	238 (94%)	14 (6%)	2 (1%)	16	30
1	DDD	255/272 (94%)	245 (96%)	10 (4%)	0	100	100
1	EEE	255/272 (94%)	242 (95%)	13 (5%)	0	100	100
1	FFF	255/272 (94%)	244 (96%)	11 (4%)	0	100	100
1	GGG	254/272 (93%)	243 (96%)	10 (4%)	1 (0%)	30	50
1	HHH	254/272 (93%)	242 (95%)	12 (5%)	0	100	100
1	III	255/272 (94%)	241 (94%)	14 (6%)	0	100	100
1	JJJ	255/272 (94%)	244 (96%)	11 (4%)	0	100	100
2	KKK	208/404 (52%)	195 (94%)	11 (5%)	2 (1%)	12	24
2	MMM	185/404 (46%)	176 (95%)	9 (5%)	0	100	100
2	OOO	211/404 (52%)	202 (96%)	8 (4%)	1 (0%)	24	43
2	QQQ	209/404 (52%)	200 (96%)	8 (4%)	1 (0%)	24	43
2	TTT	210/404 (52%)	201 (96%)	9 (4%)	0	100	100
2	VVV	208/404 (52%)	197 (95%)	9 (4%)	2 (1%)	12	24
2	XXX	197/404 (49%)	190 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	YYY	208/404 (52%)	200 (96%)	8 (4%)	0	100	100
2	bbb	211/404 (52%)	201 (95%)	9 (4%)	1 (0%)	24	43
2	ccc	196/404 (48%)	185 (94%)	11 (6%)	0	100	100
3	LLL	209/212 (99%)	195 (93%)	13 (6%)	1 (0%)	24	43
3	NNN	151/212 (71%)	134 (89%)	13 (9%)	4 (3%)	4	7
3	PPP	209/212 (99%)	192 (92%)	14 (7%)	3 (1%)	9	17
3	RRR	198/212 (93%)	186 (94%)	11 (6%)	1 (0%)	24	43
3	SSS	193/212 (91%)	177 (92%)	14 (7%)	2 (1%)	12	24
3	UUU	163/212 (77%)	148 (91%)	15 (9%)	0	100	100
3	WWW	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	24	43
3	ZZZ	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
3	aaa	209/212 (99%)	196 (94%)	12 (6%)	1 (0%)	24	43
3	ddd	202/212 (95%)	191 (95%)	9 (4%)	2 (1%)	12	24
All	All	6542/8880 (74%)	6183 (94%)	334 (5%)	25 (0%)	30	50

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	LLL	7	SER
3	NNN	7	SER
3	RRR	8	PRO
3	SSS	7	SER
3	WWW	7	SER
3	aaa	7	SER
2	bbb	2	VAL
3	ddd	7	SER
1	CCC	52	GLU
1	CCC	181	MET
2	KKK	196	SER
3	NNN	138	ASN
2	OOO	178	ALA
2	QQQ	182	SER
3	SSS	108	ARG
3	NNN	141	PRO
3	NNN	181	LEU
2	VVV	124	ALA
2	VVV	182	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	GGG	181	MET
2	KKK	195	PRO
3	PPP	7	SER
3	PPP	190	LYS
3	ddd	15	VAL
3	PPP	191	VAL

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	AAA	225/237 (95%)	221 (98%)	4 (2%)	51	71
1	BBB	225/237 (95%)	219 (97%)	6 (3%)	39	62
1	CCC	225/237 (95%)	221 (98%)	4 (2%)	51	71
1	DDD	227/237 (96%)	225 (99%)	2 (1%)	70	82
1	EEE	228/237 (96%)	224 (98%)	4 (2%)	51	71
1	FFF	226/237 (95%)	220 (97%)	6 (3%)	39	62
1	GGG	227/237 (96%)	225 (99%)	2 (1%)	70	82
1	HHH	224/237 (94%)	216 (96%)	8 (4%)	31	55
1	III	226/237 (95%)	222 (98%)	4 (2%)	51	71
1	JJJ	226/237 (95%)	222 (98%)	4 (2%)	51	71
2	KKK	176/353 (50%)	172 (98%)	4 (2%)	44	66
2	MMM	147/353 (42%)	144 (98%)	3 (2%)	48	69
2	OOO	173/353 (49%)	165 (95%)	8 (5%)	24	45
2	QQQ	168/353 (48%)	160 (95%)	8 (5%)	23	44
2	TTT	170/353 (48%)	163 (96%)	7 (4%)	27	49
2	VVV	173/353 (49%)	171 (99%)	2 (1%)	63	78
2	XXX	160/353 (45%)	158 (99%)	2 (1%)	61	76
2	YYY	174/353 (49%)	170 (98%)	4 (2%)	44	66
2	bbb	172/353 (49%)	166 (96%)	6 (4%)	32	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	ccc	162/353 (46%)	159 (98%)	3 (2%)	50	70
3	LLL	180/187 (96%)	175 (97%)	5 (3%)	38	61
3	NNN	131/187 (70%)	126 (96%)	5 (4%)	29	52
3	PPP	174/187 (93%)	169 (97%)	5 (3%)	37	61
3	RRR	173/187 (92%)	165 (95%)	8 (5%)	24	45
3	SSS	171/187 (91%)	169 (99%)	2 (1%)	63	78
3	UUU	155/187 (83%)	152 (98%)	3 (2%)	50	70
3	WWW	182/187 (97%)	177 (97%)	5 (3%)	39	62
3	ZZZ	186/187 (100%)	178 (96%)	8 (4%)	26	47
3	aaa	182/187 (97%)	177 (97%)	5 (3%)	39	62
3	ddd	180/187 (96%)	175 (97%)	5 (3%)	38	61
All	All	5648/7770 (73%)	5506 (98%)	142 (2%)	42	64

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	51	ASP
1	AAA	84	ARG
1	AAA	129	ASP
1	AAA	220	GLU
1	BBB	34	ASP
1	BBB	37	THR
1	BBB	40	GLU
1	BBB	51	ASP
1	BBB	62	SER
1	BBB	199	CYS
1	CCC	51	ASP
1	CCC	84	ARG
1	CCC	220	GLU
1	CCC	285	ARG
1	DDD	62	SER
1	DDD	222	VAL
1	EEE	24	VAL
1	EEE	34	ASP
1	EEE	99	ILE
1	EEE	201	VAL
1	FFF	34	ASP
1	FFF	41	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	FFF	62	SER
1	FFF	159	ASN
1	FFF	217	THR
1	FFF	287	VAL
1	GGG	99	ILE
1	GGG	288	LYS
1	HHH	34	ASP
1	HHH	35	SER
1	HHH	41	CYS
1	HHH	51	ASP
1	HHH	129	ASP
1	HHH	166	ASP
1	HHH	216	LEU
1	HHH	285	ARG
1	III	34	ASP
1	III	51	ASP
1	III	163	LYS
1	III	285	ARG
1	JJJ	62	SER
1	JJJ	120	VAL
1	JJJ	163	LYS
1	JJJ	216	LEU
2	KKK	96	CYS
2	KKK	125	SER
2	KKK	183	SER
2	KKK	209	ASN
3	LLL	9	SER
3	LLL	11	LEU
3	LLL	18	ARG
3	LLL	56	SER
3	LLL	206	THR
2	MMM	54	ASP
2	MMM	163	SER
2	MMM	190	SER
3	NNN	54	LEU
3	NNN	63	SER
3	NNN	109	THR
3	NNN	162	SER
3	NNN	178	THR
2	OOO	54	ASP
2	OOO	89	GLU
2	OOO	130	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	OOO	170	THR
2	OOO	179	VAL
2	OOO	196	SER
2	OOO	197	SER
2	OOO	201	THR
3	PPP	5	THR
3	PPP	9	SER
3	PPP	53	THR
3	PPP	56	SER
3	PPP	176	SER
2	QQQ	7	SER
2	QQQ	13	GLN
2	QQQ	28	THR
2	QQQ	123	SER
2	QQQ	148	LEU
2	QQQ	179	VAL
2	QQQ	180	LEU
2	QQQ	197	SER
3	RRR	7	SER
3	RRR	8	PRO
3	RRR	9	SER
3	RRR	52	SER
3	RRR	178	THR
3	RRR	199	GLN
3	RRR	202	SER
3	RRR	204	PRO
3	SSS	26	SER
3	SSS	105	ASP
2	TTT	73	ASP
2	TTT	96	CYS
2	TTT	145	THR
2	TTT	158	GLU
2	TTT	170	THR
2	TTT	207	ASN
2	TTT	219	LYS
3	UUU	5	THR
3	UUU	152	ASN
3	UUU	199	GLN
2	VVV	96	CYS
2	VVV	201	THR
3	WWW	5	THR
3	WWW	9	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	WWW	126	LYS
3	WWW	180	THR
3	WWW	202	SER
2	XXX	89	GLU
2	XXX	170	THR
2	YYY	127	LYS
2	YYY	160	VAL
2	YYY	171	SER
2	YYY	196	SER
3	ZZZ	20	THR
3	ZZZ	114	SER
3	ZZZ	142	ARG
3	ZZZ	154	LEU
3	ZZZ	156	SER
3	ZZZ	162	SER
3	ZZZ	179	LEU
3	ZZZ	208	SER
3	aaa	10	SER
3	aaa	108	ARG
3	aaa	109	THR
3	aaa	168	SER
3	aaa	208	SER
2	bbb	96	CYS
2	bbb	170	THR
2	bbb	197	SER
2	bbb	198	SER
2	bbb	203	THR
2	bbb	214	ASN
2	ccc	21	SER
2	ccc	120	THR
2	ccc	125	SER
3	ddd	9	SER
3	ddd	11	LEU
3	ddd	124	GLN
3	ddd	154	LEU
3	ddd	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	AAA	259/272 (95%)	-0.28	6 (2%) 61 59	26, 37, 57, 83	0
1	BBB	258/272 (94%)	-0.36	3 (1%) 76 76	24, 36, 55, 92	0
1	CCC	258/272 (94%)	-0.41	1 (0%) 88 89	23, 32, 53, 72	0
1	DDD	259/272 (95%)	-0.45	5 (1%) 66 64	23, 31, 50, 73	0
1	EEE	259/272 (95%)	-0.41	2 (0%) 82 82	24, 34, 54, 81	0
1	FFF	259/272 (95%)	-0.39	3 (1%) 76 76	23, 34, 53, 88	0
1	GGG	258/272 (94%)	-0.46	3 (1%) 76 76	23, 31, 51, 81	0
1	HHH	258/272 (94%)	-0.41	4 (1%) 70 69	22, 33, 53, 80	0
1	III	259/272 (95%)	-0.37	3 (1%) 76 76	25, 35, 55, 84	0
1	JJJ	259/272 (95%)	-0.40	1 (0%) 88 89	23, 35, 56, 82	0
2	KKK	214/404 (52%)	0.02	5 (2%) 61 59	23, 48, 79, 96	0
2	MMM	191/404 (47%)	0.25	5 (2%) 57 55	34, 57, 82, 91	0
2	OOO	215/404 (53%)	0.15	2 (0%) 81 81	25, 54, 77, 90	0
2	QQQ	213/404 (52%)	0.44	10 (4%) 36 36	30, 64, 95, 103	0
2	TTT	214/404 (52%)	0.38	5 (2%) 61 59	34, 61, 82, 99	0
2	VVV	212/404 (52%)	0.03	3 (1%) 73 73	32, 52, 83, 101	0
2	XXX	203/404 (50%)	0.18	12 (5%) 28 28	23, 50, 107, 129	0
2	YYY	212/404 (52%)	0.14	3 (1%) 73 73	25, 54, 81, 96	0
2	bbb	215/404 (53%)	0.03	5 (2%) 61 59	27, 51, 74, 84	0
2	ccc	202/404 (50%)	0.24	9 (4%) 38 37	26, 58, 83, 96	0
3	LLL	211/212 (99%)	0.19	1 (0%) 87 87	27, 59, 85, 112	0
3	NNN	157/212 (74%)	0.59	16 (10%) 12 11	33, 64, 100, 119	0
3	PPP	211/212 (99%)	0.33	3 (1%) 73 73	29, 57, 98, 108	0
3	RRR	202/212 (95%)	0.70	12 (5%) 28 28	29, 75, 100, 116	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	SSS	199/212 (93%)	0.35	4 (2%) 65 63	31, 60, 94, 108	0
3	UUU	175/212 (82%)	0.36	15 (8%) 16 16	28, 53, 105, 128	0
3	WWW	212/212 (100%)	0.36	8 (3%) 44 41	32, 60, 92, 107	0
3	ZZZ	211/212 (99%)	0.36	8 (3%) 44 41	29, 58, 96, 113	0
3	aaa	211/212 (99%)	0.50	13 (6%) 26 26	28, 64, 100, 113	0
3	ddd	206/212 (97%)	0.61	16 (7%) 19 19	26, 67, 98, 119	0
All	All	6672/8880 (75%)	0.03	186 (2%) 55 53	22, 46, 89, 129	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	KKK	140	SER	5.6
3	NNN	183	LYS	4.8
3	NNN	179	LEU	4.2
2	TTT	211	LYS	4.1
3	ddd	134	CYS	3.9
3	UUU	150	VAL	3.9
1	DDD	289	ASN	3.9
2	XXX	132	PHE	3.8
3	UUU	130	ALA	3.7
1	FFF	33	VAL	3.7
3	aaa	118	PHE	3.6
3	SSS	153	ALA	3.6
1	III	33	VAL	3.5
3	SSS	209	PHE	3.5
3	UUU	155	GLN	3.5
1	GGG	24	VAL	3.5
3	UUU	205	VAL	3.5
3	NNN	141	PRO	3.5
2	bbb	145	THR	3.4
1	JJJ	99	ILE	3.4
2	ccc	148	LEU	3.3
1	GGG	288	LYS	3.3
2	ccc	135	ALA	3.3
2	XXX	168	ALA	3.2
1	GGG	99	ILE	3.2
3	RRR	205	VAL	3.2
1	EEE	99	ILE	3.1
1	III	24	VAL	3.1
3	UUU	154	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	UUU	120	PRO	3.1
2	MMM	132	PHE	3.1
3	RRR	83	PHE	3.1
2	MMM	28	THR	3.1
3	PPP	154	LEU	3.0
3	aaa	81	GLU	3.0
2	ccc	195	PRO	3.0
3	NNN	117	ILE	3.0
2	XXX	194	VAL	3.0
3	aaa	142	ARG	3.0
1	DDD	90	LEU	3.0
2	XXX	151	LEU	3.0
3	PPP	203	SER	3.0
3	aaa	194	CYS	3.0
2	XXX	133	PRO	2.9
2	QQQ	54	ASP	2.9
2	bbb	135	ALA	2.9
2	XXX	205	ILE	2.9
1	DDD	24	VAL	2.9
1	EEE	33	VAL	2.9
3	WWW	212	GLY	2.9
2	QQQ	175	THR	2.9
3	NNN	110	VAL	2.9
2	TTT	43	LYS	2.8
3	ZZZ	180	THR	2.8
1	AAA	289	ASN	2.8
3	ddd	186	TYR	2.8
3	NNN	118	PHE	2.8
2	YYY	2	VAL	2.8
2	YYY	146	ALA	2.8
1	FFF	99	ILE	2.8
3	UUU	132	VAL	2.7
1	III	32	GLY	2.7
2	OOO	54	ASP	2.7
3	NNN	116	PHE	2.7
3	ZZZ	184	ALA	2.7
3	SSS	185	ASP	2.7
1	AAA	99	ILE	2.6
2	VVV	123	SER	2.6
3	WWW	184	ALA	2.6
3	RRR	181	LEU	2.6
1	HHH	33	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	ccc	170	THR	2.6
3	NNN	134	CYS	2.6
3	NNN	182	SER	2.6
1	AAA	33	VAL	2.6
1	BBB	33	VAL	2.6
2	MMM	170	THR	2.5
1	HHH	51	ASP	2.5
2	MMM	172	GLY	2.5
2	XXX	219	LYS	2.5
3	aaa	145	LYS	2.5
3	ddd	173	TYR	2.5
3	NNN	120	PRO	2.5
3	NNN	144	ALA	2.5
3	aaa	133	VAL	2.5
3	UUU	129	THR	2.5
3	UUU	158	ASN	2.5
3	NNN	108	ARG	2.5
2	XXX	208	VAL	2.5
3	RRR	110	VAL	2.5
2	YYY	112	PHE	2.5
2	KKK	145	THR	2.4
3	RRR	178	THR	2.4
1	BBB	91	ASN	2.4
2	XXX	167	GLY	2.4
2	TTT	216	LYS	2.4
2	ccc	194	VAL	2.4
3	ZZZ	126	LYS	2.4
3	ddd	110	VAL	2.4
3	UUU	153	ALA	2.4
1	HHH	289	ASN	2.4
2	TTT	86	LEU	2.4
2	QQQ	190	SER	2.4
3	SSS	205	VAL	2.4
2	VVV	199	LEU	2.4
3	RRR	7	SER	2.4
3	aaa	148	TRP	2.4
1	BBB	99	ILE	2.4
1	FFF	289	ASN	2.4
3	PPP	211	ARG	2.4
3	RRR	132	VAL	2.4
3	ZZZ	129	THR	2.3
3	NNN	123	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	ddd	113	PRO	2.3
2	XXX	221	VAL	2.3
2	ccc	192	VAL	2.3
2	KKK	170	THR	2.3
2	VVV	195	PRO	2.3
2	MMM	96	CYS	2.3
1	AAA	24	VAL	2.3
2	ccc	221	VAL	2.3
3	ddd	146	VAL	2.3
2	KKK	148	LEU	2.3
2	QQQ	148	LEU	2.3
3	RRR	153	ALA	2.3
3	RRR	154	LEU	2.3
3	ddd	180	THR	2.3
3	WWW	157	GLY	2.3
3	aaa	154	LEU	2.3
2	QQQ	145	THR	2.3
3	WWW	183	LYS	2.3
1	HHH	288	LYS	2.2
3	RRR	192	TYR	2.2
3	UUU	119	PRO	2.2
3	ddd	192	TYR	2.2
3	LLL	159	SER	2.2
3	aaa	177	SER	2.2
3	ddd	78	LEU	2.2
3	aaa	146	VAL	2.2
2	QQQ	203	THR	2.2
3	WWW	186	TYR	2.2
3	NNN	181	LEU	2.2
3	UUU	175	LEU	2.2
3	ZZZ	177	SER	2.2
2	QQQ	132	PHE	2.2
2	bbb	223	PRO	2.2
2	ccc	204	TYR	2.2
2	TTT	44	GLY	2.2
3	ddd	157	GLY	2.2
3	NNN	115	VAL	2.2
3	ZZZ	153	ALA	2.1
3	ddd	137	ASN	2.1
3	ddd	136	LEU	2.1
3	UUU	131	SER	2.1
3	WWW	146	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	aaa	132	VAL	2.1
3	ddd	174	SER	2.1
3	aaa	204	PRO	2.1
3	WWW	181	LEU	2.1
3	UUU	196	VAL	2.1
2	ccc	147	ALA	2.1
3	ddd	112	ALA	2.1
3	WWW	126	LYS	2.1
3	ZZZ	8	PRO	2.1
3	ddd	204	PRO	2.1
2	QQQ	188	LEU	2.1
1	CCC	99	ILE	2.1
1	DDD	33	VAL	2.1
2	QQQ	124	ALA	2.1
3	ZZZ	201	LEU	2.1
1	AAA	35	SER	2.0
2	OOO	43	LYS	2.0
2	KKK	195	PRO	2.0
3	UUU	8	PRO	2.0
2	XXX	134	LEU	2.0
2	XXX	169	LEU	2.0
2	bbb	134	LEU	2.0
1	AAA	32	GLY	2.0
1	DDD	99	ILE	2.0
2	QQQ	12	VAL	2.0
2	bbb	132	PHE	2.0
3	aaa	126	LYS	2.0
3	NNN	178	THR	2.0
3	RRR	11	LEU	2.0
3	ddd	175	LEU	2.0
3	RRR	157	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.