



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 05:19 PM EDT

PDB ID : 2Z0L  
Title : Crystal structure of EBV-DNA polymerase accessory protein BMRF1  
Authors : Murayama, K.; Kato-Murayama, M.; Terada, T.; Shirouzu, M.; Yokoyama, S.;  
RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-05-07  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

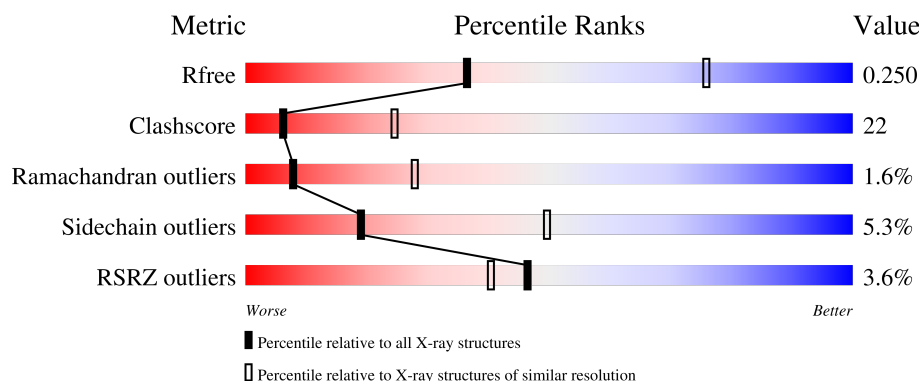
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	 2% 59% 32% 6%
1	B	318	 4% 57% 33% 6%
1	C	318	 3% 61% 28% 6%
1	D	318	 6% 58% 33% 6%
1	E	318	 3% 55% 36% 6%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	318	<div><div></div><div>3%</div><div>64%</div><div>28%</div><div>6%</div></div>
1	G	318	<div><div></div><div>4%</div><div>55%</div><div>36%</div><div>6%</div></div>
1	H	318	<div><div></div><div>4%</div><div>59%</div><div>31%</div><div>6%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18098 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 Early antigen protein D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	B	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	C	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	D	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	E	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	F	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	G	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			
1	H	299	Total	C	N	O	S	Se	0	0	0
			2246	1425	387	422	6	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P03191
A	-2	SER	-	expression tag	UNP P03191
A	-1	SER	-	expression tag	UNP P03191
A	0	GLY	-	expression tag	UNP P03191
B	-3	GLY	-	expression tag	UNP P03191
B	-2	SER	-	expression tag	UNP P03191
B	-1	SER	-	expression tag	UNP P03191
B	0	GLY	-	expression tag	UNP P03191
C	-3	GLY	-	expression tag	UNP P03191
C	-2	SER	-	expression tag	UNP P03191
C	-1	SER	-	expression tag	UNP P03191
C	0	GLY	-	expression tag	UNP P03191
D	-3	GLY	-	expression tag	UNP P03191

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP P03191
D	-1	SER	-	expression tag	UNP P03191
D	0	GLY	-	expression tag	UNP P03191
E	-3	GLY	-	expression tag	UNP P03191
E	-2	SER	-	expression tag	UNP P03191
E	-1	SER	-	expression tag	UNP P03191
E	0	GLY	-	expression tag	UNP P03191
F	-3	GLY	-	expression tag	UNP P03191
F	-2	SER	-	expression tag	UNP P03191
F	-1	SER	-	expression tag	UNP P03191
F	0	GLY	-	expression tag	UNP P03191
G	-3	GLY	-	expression tag	UNP P03191
G	-2	SER	-	expression tag	UNP P03191
G	-1	SER	-	expression tag	UNP P03191
G	0	GLY	-	expression tag	UNP P03191
H	-3	GLY	-	expression tag	UNP P03191
H	-2	SER	-	expression tag	UNP P03191
H	-1	SER	-	expression tag	UNP P03191
H	0	GLY	-	expression tag	UNP P03191

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	C	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	3	Total Cl 3 3	0	0
2	H	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	21	Total O 21 21	0	0

*Continued on next page...*

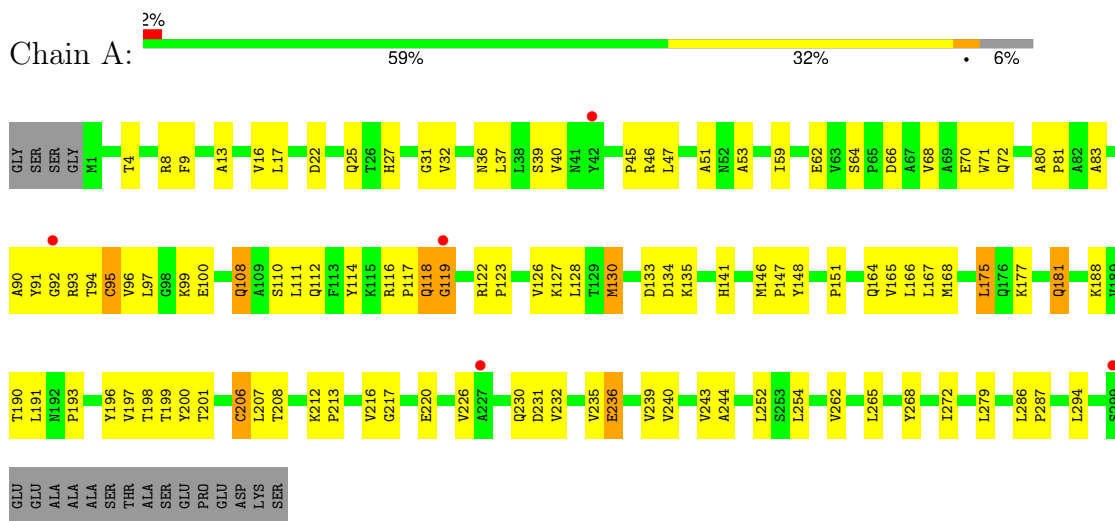
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	12	Total 12	O 12	0	0
3	D	9	Total 9	O 9	0	0
3	E	10	Total 10	O 10	0	0
3	F	19	Total 19	O 19	0	0
3	G	20	Total 20	O 20	0	0
3	H	17	Total 17	O 17	0	0

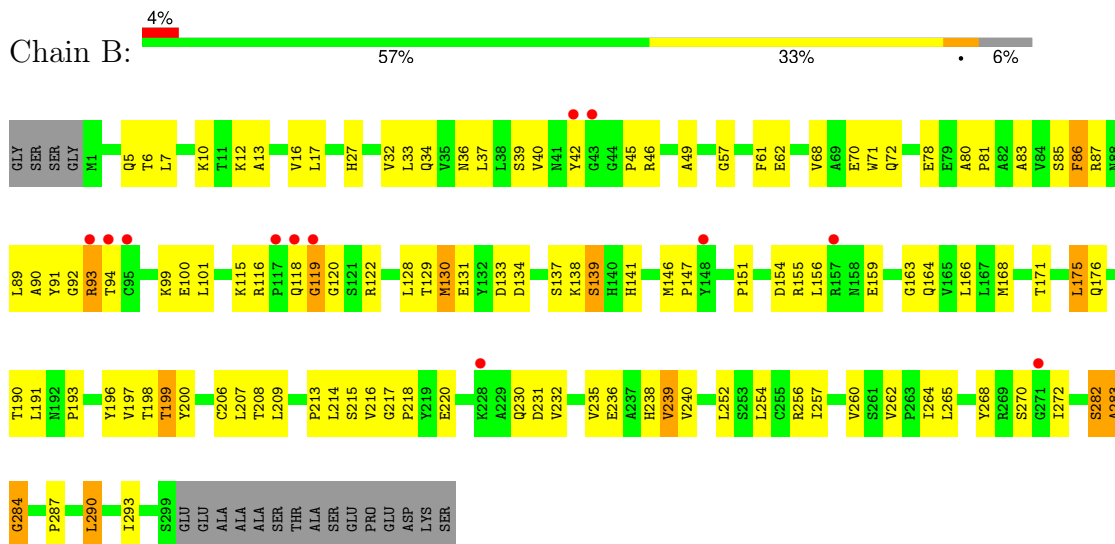
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Early antigen protein D

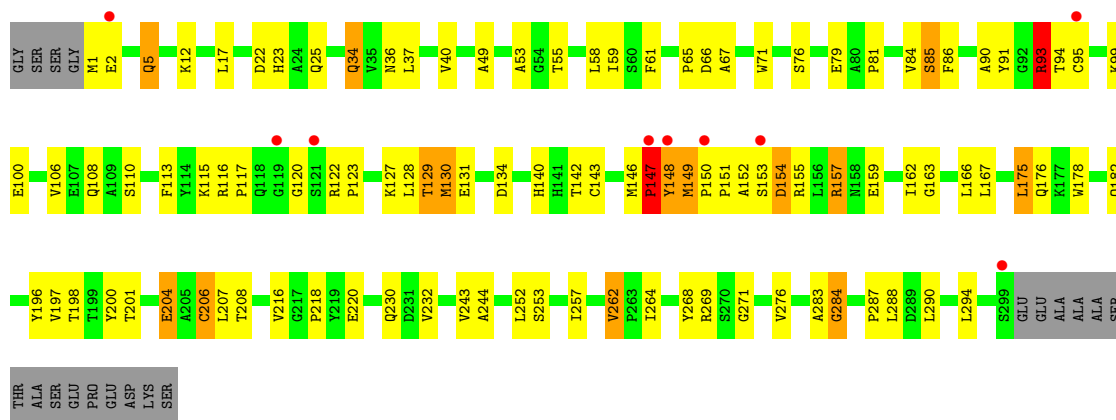


- Molecule 1: Early antigen protein D

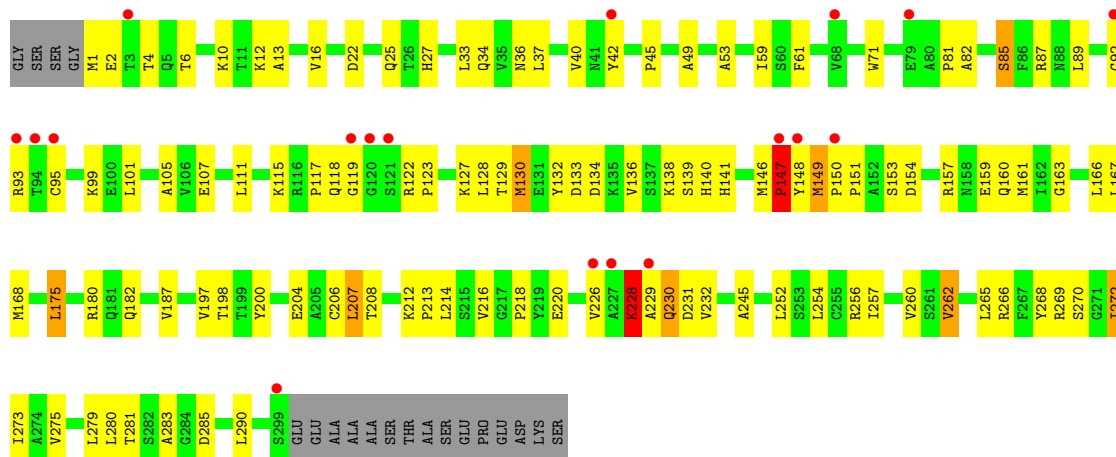


- Molecule 1: Early antigen protein D

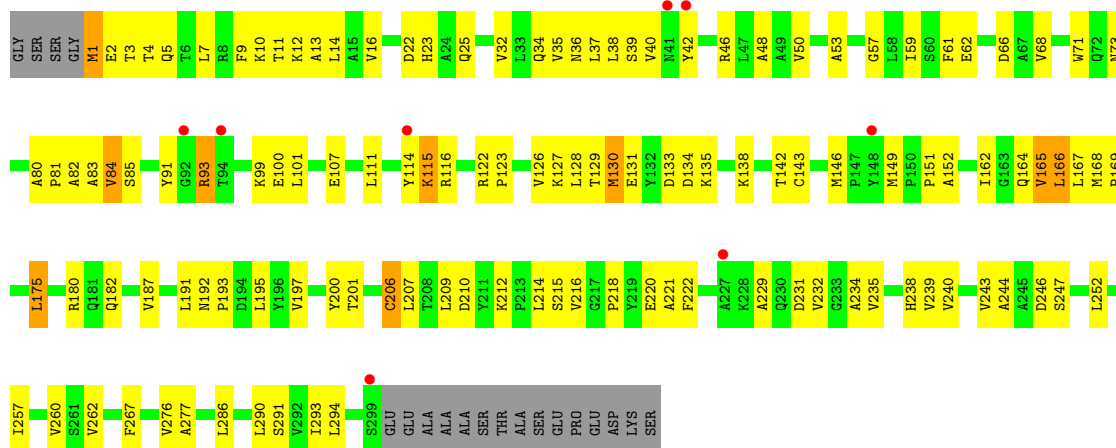




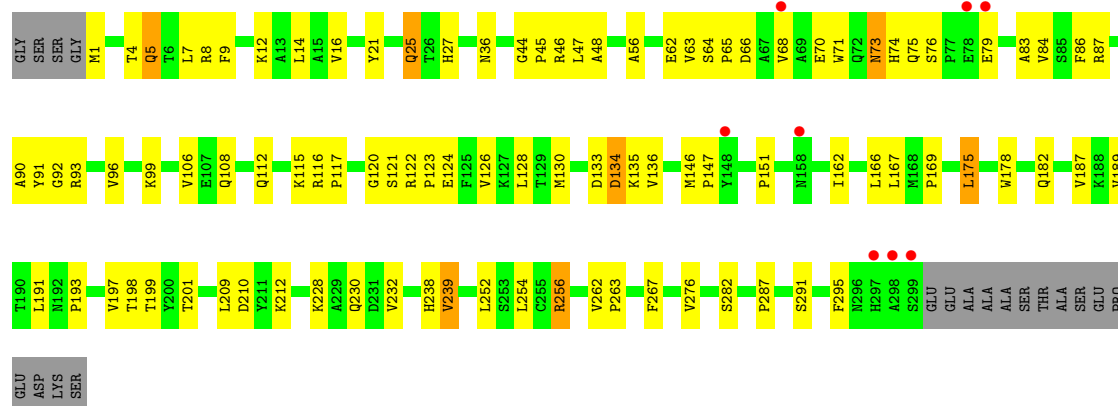
• Molecule 1: Early antigen protein D



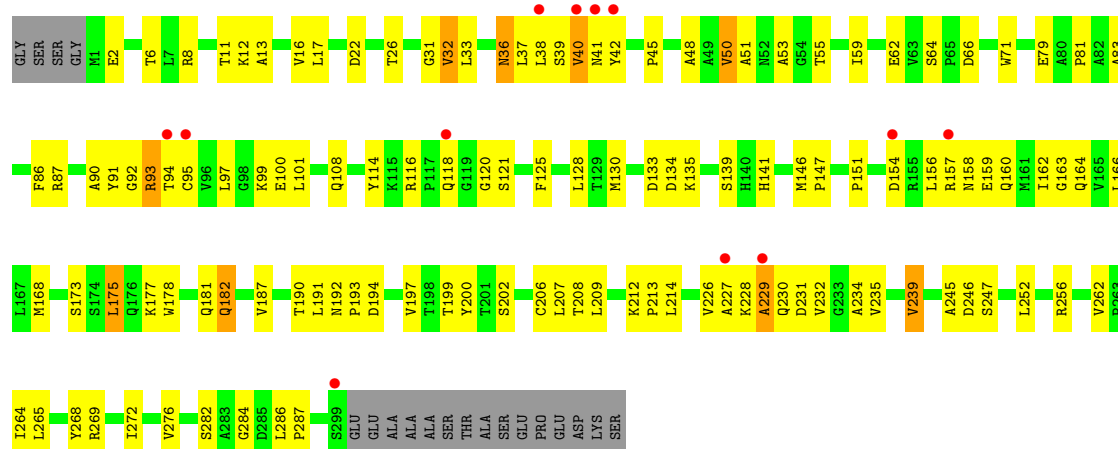
• Molecule 1: Early antigen protein D



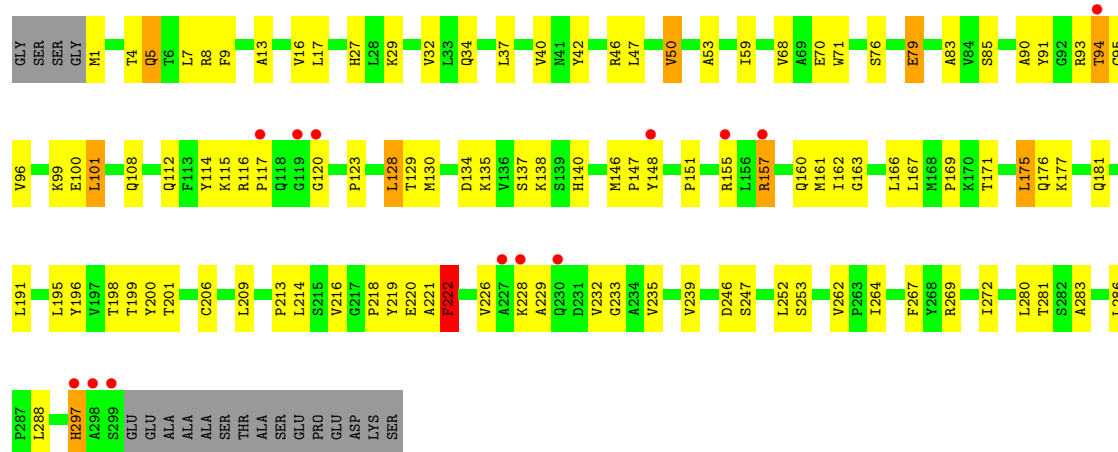
• Molecule 1: Early antigen protein D



• Molecule 1: Early antigen protein D



• Molecule 1: Early antigen protein D



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.67Å 191.63Å 371.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.90 48.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-2.90) 99.4 (48.38-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.251 0.206 , 0.250	Depositor DCC
$R_{free}$ test set	9872 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

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	0.40	0/2288	0.65	0/3105
1	B	0.42	0/2288	0.71	0/3105
1	C	0.50	3/2288 (0.1%)	0.74	3/3105 (0.1%)
1	D	0.49	1/2288 (0.0%)	0.76	3/3105 (0.1%)
1	E	0.38	0/2288	0.65	0/3105
1	F	0.39	0/2288	0.67	0/3105
1	G	0.42	0/2288	0.69	0/3105
1	H	0.39	0/2288	0.70	0/3105
All	All	0.43	4/18304 (0.0%)	0.70	6/24840 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	118	GLN	C-N	-6.02	1.22	1.33
1	C	147	PRO	CA-C	-5.88	1.41	1.52
1	C	147	PRO	C-N	-5.45	1.21	1.34
1	C	148	TYR	N-CA	-5.33	1.35	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	PRO	CA-N-CD	-8.45	99.68	111.50
1	C	147	PRO	C-N-CA	-6.94	104.36	121.70
1	D	147	PRO	C-N-CA	-5.83	107.13	121.70
1	C	147	PRO	N-CA-CB	5.61	110.04	103.30
1	D	228	LYS	N-CA-C	5.35	125.45	111.00
1	D	147	PRO	CA-N-CD	-5.03	104.46	111.50

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	2246	0	2265	97	0
1	B	2246	0	2265	105	0
1	C	2246	0	2265	97	0
1	D	2246	0	2265	105	0
1	E	2246	0	2267	126	0
1	F	2246	0	2267	86	0
1	G	2246	0	2267	111	0
1	H	2246	0	2267	97	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	1	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	0	0	0
3	B	21	0	0	0	0
3	C	12	0	0	1	0
3	D	9	0	0	0	0
3	E	10	0	0	0	0
3	F	19	0	0	2	0
3	G	20	0	0	4	0
3	H	17	0	0	2	0
All	All	18098	0	18128	793	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 22.

All (793) 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:B:168:MSE:HE3	1:B:231:ASP:H	1.28	0.98
1:A:116:ARG:HB3	1:A:118:GLN:HE21	1.31	0.96
1:D:87:ARG:HB3	1:D:146:MSE:HE3	1.51	0.92
1:A:32:VAL:HG11	1:A:146:MSE:HE1	1.52	0.92
1:A:99:LYS:HD2	1:B:94:THR:HG21	1.52	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LEU:HB3	1:D:130:MSE:HE1	1.54	0.90
1:C:90:ALA:HB3	1:C:93:ARG:HG3	1.53	0.89
1:D:226:VAL:HG23	1:D:280:LEU:HD23	1.54	0.89
1:F:175:LEU:HD13	1:F:252:LEU:HD11	1.53	0.89
1:E:111:LEU:HG	1:E:128:LEU:HD23	1.55	0.88
1:E:38:LEU:HD11	1:E:82:ALA:HB1	1.56	0.87
1:D:228:LYS:HG2	1:D:229:ALA:N	1.87	0.87
1:D:270:SER:HB3	1:D:272:ILE:HG22	1.54	0.87
1:B:191:LEU:HD21	1:B:235:VAL:HG13	1.54	0.86
1:D:2:GLU:HG3	1:D:117:PRO:HA	1.57	0.86
1:C:36:ASN:HD22	1:C:153:SER:HB2	1.42	0.84
1:H:216:VAL:HB	1:H:220:GLU:HB2	1.59	0.84
1:G:83:ALA:HB2	1:G:151:PRO:HG3	1.60	0.83
1:B:175:LEU:HD13	1:B:252:LEU:HD11	1.61	0.83
1:C:122:ARG:HD2	1:C:148:TYR:CZ	2.13	0.83
1:C:162:ILE:HD11	1:C:269:ARG:HG2	1.62	0.82
1:H:157:ARG:HB3	1:H:157:ARG:HH11	1.45	0.81
1:C:230:GLN:HG3	1:C:232:VAL:HG23	1.63	0.81
1:D:161:MSE:HE1	1:D:266:ARG:HD3	1.62	0.80
1:E:34:GLN:HG3	1:E:85:SER:HB3	1.65	0.79
1:E:131:GLU:HG2	1:E:138:LYS:HE2	1.65	0.78
1:C:122:ARG:HD2	1:C:148:TYR:CE2	2.19	0.78
1:C:86:PHE:HA	1:C:146:MSE:HG2	1.64	0.78
1:A:100:GLU:HB3	1:A:130:MSE:HE2	1.66	0.78
1:B:37:LEU:O	1:B:40:VAL:HG23	1.84	0.78
1:B:196:TYR:HD2	1:B:213:PRO:HG3	1.49	0.77
1:G:17:LEU:HD21	1:G:287:PRO:HD2	1.67	0.77
1:E:83:ALA:HB2	1:E:151:PRO:HG3	1.67	0.76
1:C:122:ARG:HG3	1:C:148:TYR:OH	1.85	0.76
1:E:168:MSE:HA	1:E:229:ALA:HB1	1.65	0.76
1:A:83:ALA:HB2	1:A:151:PRO:HG3	1.66	0.76
1:A:32:VAL:CG1	1:A:146:MSE:HE1	2.14	0.76
1:H:226:VAL:HG12	1:H:228:LYS:O	1.86	0.76
1:B:49:ALA:HB3	1:B:61:PHE:HB3	1.67	0.76
1:C:243:VAL:HG11	1:C:294:LEU:HD13	1.67	0.75
1:G:139:SER:HB3	1:H:93:ARG:HH21	1.50	0.75
1:D:22:ASP:O	1:D:25:GLN:HG2	1.87	0.75
1:G:191:LEU:HB3	1:G:239:VAL:HG23	1.69	0.75
1:H:34:GLN:HB3	1:H:85:SER:HB3	1.69	0.74
1:A:175:LEU:HD13	1:A:252:LEU:HD11	1.70	0.74
1:B:90:ALA:HB3	1:B:93:ARG:HG3	1.69	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ALA:HB2	1:F:151:PRO:HG3	1.70	0.73
1:D:37:LEU:HD12	1:D:81:PRO:O	1.88	0.73
1:D:161:MSE:CE	1:D:266:ARG:HD3	2.19	0.73
1:H:155:ARG:NH2	1:H:272:ILE:HD11	2.04	0.73
1:A:196:TYR:CD2	1:A:213:PRO:HG3	2.23	0.73
1:H:7:LEU:HD13	1:H:71:TRP:CE3	2.24	0.72
1:F:96:VAL:HG23	1:F:99:LYS:HB2	1.70	0.72
1:G:36:ASN:ND2	1:G:38:LEU:H	1.85	0.72
1:F:64:SER:HB2	1:F:66:ASP:OD2	1.89	0.72
1:H:175:LEU:HD13	1:H:252:LEU:HD11	1.71	0.72
1:E:22:ASP:O	1:E:25:GLN:HG2	1.89	0.72
1:H:201:THR:HG22	1:H:206:CYS:HB3	1.70	0.72
1:D:129:THR:C	1:D:130:MSE:HE3	2.10	0.72
1:F:48:ALA:HB2	1:F:62:GLU:HB3	1.72	0.72
1:H:128:LEU:HD12	1:H:128:LEU:H	1.55	0.72
1:A:96:VAL:HG22	1:A:99:LYS:HB2	1.72	0.72
1:D:270:SER:HB3	1:D:272:ILE:CG2	2.20	0.72
1:G:86:PHE:HA	1:G:146:MSE:HG3	1.72	0.71
1:B:196:TYR:CD2	1:B:213:PRO:HG3	2.25	0.71
1:B:115:LYS:HD3	1:B:120:GLY:O	1.91	0.71
1:B:168:MSE:HE3	1:B:231:ASP:N	2.05	0.70
1:D:138:LYS:HE2	1:D:140:HIS:CE1	2.26	0.70
1:H:157:ARG:HB3	1:H:157:ARG:NH1	2.04	0.70
1:E:1:MSE:HG2	1:E:114:TYR:CD1	2.27	0.70
1:G:48:ALA:HB2	1:G:62:GLU:HG2	1.74	0.70
1:A:116:ARG:HB3	1:A:118:GLN:NE2	2.06	0.70
1:E:216:VAL:HG22	1:E:220:GLU:HB2	1.74	0.69
1:H:76:SER:HB3	1:H:79:GLU:HB2	1.74	0.69
1:C:49:ALA:HB3	1:C:61:PHE:HB3	1.75	0.69
1:G:32:VAL:HG12	1:G:50:VAL:HG13	1.74	0.69
1:H:7:LEU:HD13	1:H:71:TRP:HE3	1.58	0.69
1:H:100:GLU:HB2	1:H:130:MSE:HE2	1.75	0.69
1:H:160:GLN:OE1	1:H:269:ARG:HD2	1.93	0.69
1:D:40:VAL:HG22	1:D:45:PRO:HG3	1.75	0.68
1:D:53:ALA:HB2	1:D:59:ILE:HD11	1.73	0.68
1:H:1:MSE:HE1	1:H:116:ARG:HA	1.76	0.68
1:A:96:VAL:CG2	1:A:99:LYS:HB2	2.24	0.68
1:G:37:LEU:O	1:G:40:VAL:HG13	1.94	0.68
1:E:1:MSE:HE3	1:E:1:MSE:HA	1.75	0.68
1:F:87:ARG:HH21	1:F:146:MSE:HE3	1.59	0.68
1:H:1:MSE:HE1	1:H:116:ARG:HG2	1.76	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:HG3	1:C:142:THR:HG22	1.75	0.67
1:D:128:LEU:CB	1:D:130:MSE:HE1	2.23	0.67
1:D:111:LEU:HD23	1:D:128:LEU:HG	1.75	0.67
1:E:286:LEU:HD12	1:E:286:LEU:H	1.58	0.67
1:A:8:ARG:HD2	1:A:108:GLN:OE1	1.95	0.67
1:D:268:TYR:HB2	1:D:272:ILE:HG23	1.77	0.67
1:A:94:THR:HG21	1:B:99:LYS:HE3	1.77	0.67
1:D:45:PRO:HG2	1:D:71:TRP:CD2	2.29	0.66
1:A:93:ARG:NH2	1:B:137:SER:HB3	2.11	0.66
1:B:166:LEU:HD12	1:B:264:ILE:HG12	1.77	0.66
1:C:201:THR:HG22	1:C:206:CYS:HB2	1.76	0.66
1:B:168:MSE:CE	1:B:231:ASP:H	2.06	0.66
1:C:163:GLY:HA2	1:C:218:PRO:HG3	1.78	0.66
1:B:32:VAL:HG11	1:B:146:MSE:HE1	1.77	0.66
1:A:36:ASN:ND2	1:A:151:PRO:HB3	2.12	0.65
1:C:166:LEU:HD23	1:C:167:LEU:N	2.11	0.65
1:C:90:ALA:CB	1:C:93:ARG:HG3	2.24	0.65
1:A:235:VAL:HG12	1:A:236:GLU:N	2.10	0.65
1:C:216:VAL:HB	1:C:220:GLU:HB2	1.79	0.65
1:D:168:MSE:HG2	1:D:230:GLN:H	1.61	0.65
1:H:34:GLN:CB	1:H:85:SER:HB3	2.27	0.65
1:B:13:ALA:O	1:B:16:VAL:HG22	1.96	0.65
1:G:130:MSE:HE2	3:G:511:HOH:O	1.97	0.65
1:G:37:LEU:HD22	1:G:71:TRP:HH2	1.62	0.64
1:B:27:HIS:ND1	1:B:254:LEU:HD21	2.12	0.64
1:H:1:MSE:HE2	1:H:117:PRO:HD3	1.80	0.64
1:C:122:ARG:CD	1:C:148:TYR:CZ	2.79	0.64
1:D:34:GLN:HG3	1:D:85:SER:HB3	1.79	0.64
1:A:91:TYR:C	1:A:93:ARG:H	2.01	0.64
1:F:7:LEU:HD13	1:F:71:TRP:CE3	2.32	0.64
1:B:36:ASN:ND2	1:B:151:PRO:HB3	2.13	0.63
1:C:76:SER:HB3	1:C:79:GLU:HG2	1.79	0.63
1:E:1:MSE:HE2	1:E:116:ARG:HA	1.80	0.63
1:A:22:ASP:O	1:A:25:GLN:HG2	1.99	0.63
1:H:32:VAL:HG11	1:H:146:MSE:HE1	1.80	0.63
1:E:169:PRO:HD3	1:E:229:ALA:CB	2.28	0.63
1:G:133:ASP:HB2	1:H:91:TYR:OH	1.99	0.63
1:F:73:ASN:ND2	1:F:75:GLN:H	1.97	0.63
1:G:37:LEU:HD22	1:G:71:TRP:CH2	2.33	0.63
1:H:29:LYS:HG3	1:H:96:VAL:HG21	1.80	0.63
1:G:36:ASN:HD22	1:G:37:LEU:N	1.97	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MSE:HE2	1:C:116:ARG:HA	1.80	0.62
1:G:97:LEU:HD22	1:G:128:LEU:HD22	1.81	0.62
1:B:168:MSE:HE2	1:B:230:GLN:HA	1.81	0.62
1:B:198:THR:HG22	1:B:209:LEU:HB2	1.82	0.62
1:A:96:VAL:HG23	1:A:99:LYS:H	1.65	0.62
1:B:191:LEU:HD21	1:B:235:VAL:CG1	2.27	0.62
1:D:1:MSE:HA	1:D:117:PRO:HD3	1.80	0.62
1:D:168:MSE:HG3	1:D:231:ASP:OD1	1.99	0.62
1:E:175:LEU:HD13	1:E:252:LEU:HD11	1.81	0.61
1:C:175:LEU:HD13	1:C:252:LEU:HD11	1.80	0.61
1:G:168:MSE:HG2	1:G:231:ASP:OD1	2.00	0.61
1:F:73:ASN:HD22	1:F:75:GLN:H	1.49	0.61
1:A:167:LEU:O	1:A:262:VAL:HG13	2.00	0.61
1:G:37:LEU:HD12	1:G:81:PRO:O	2.00	0.61
1:G:182:GLN:HG2	1:G:202:SER:HB3	1.81	0.61
1:G:190:THR:HB	1:G:199:THR:OG1	2.00	0.61
1:D:134:ASP:OD1	1:D:134:ASP:O	2.18	0.61
1:C:85:SER:HB2	1:C:146:MSE:HB2	1.82	0.61
1:A:207:LEU:HD12	1:D:204:GLU:O	2.01	0.61
1:D:161:MSE:HE2	1:D:266:ARG:HB3	1.83	0.60
1:E:175:LEU:HB3	1:E:252:LEU:HD13	1.82	0.60
1:C:93:ARG:HG2	1:C:93:ARG:HH11	1.66	0.60
1:G:91:TYR:O	1:G:93:ARG:N	2.28	0.60
1:C:93:ARG:HD3	1:D:132:TYR:CZ	2.36	0.60
1:D:87:ARG:HB3	1:D:146:MSE:CE	2.29	0.60
1:F:1:MSE:HE2	1:F:117:PRO:HD3	1.84	0.60
1:A:166:LEU:HD21	1:A:262:VAL:HG11	1.84	0.60
1:C:230:GLN:HG3	1:C:232:VAL:CG2	2.30	0.60
1:H:157:ARG:HH11	1:H:157:ARG:CB	2.15	0.60
1:F:96:VAL:HG23	1:F:99:LYS:CB	2.31	0.60
1:G:108:GLN:HG3	3:G:526:HOH:O	2.01	0.60
1:E:182:GLN:HA	1:E:182:GLN:NE2	2.16	0.59
1:H:191:LEU:HD13	1:H:235:VAL:HG13	1.84	0.59
1:F:87:ARG:NH2	1:F:146:MSE:HE3	2.16	0.59
1:H:196:TYR:CD2	1:H:213:PRO:HG3	2.37	0.59
1:D:36:ASN:HD22	1:D:153:SER:HB2	1.65	0.59
1:D:87:ARG:NE	1:D:89:LEU:O	2.35	0.59
1:E:127:LYS:HG3	1:E:142:THR:HG22	1.82	0.59
1:F:4:THR:HG21	1:F:123:PRO:HG3	1.83	0.59
1:B:32:VAL:CG1	1:B:146:MSE:HE1	2.33	0.59
1:G:193:PRO:HG3	1:G:235:VAL:HG11	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:TYR:HB2	1:G:272:ILE:HG22	1.84	0.59
1:H:8:ARG:HG2	1:H:108:GLN:HE22	1.67	0.59
1:H:27:HIS:HB3	1:H:59:ILE:CD1	2.33	0.59
1:H:163:GLY:HA2	1:H:218:PRO:HG3	1.84	0.59
1:D:226:VAL:HG22	1:D:279:LEU:O	2.02	0.59
1:E:37:LEU:HD22	1:E:81:PRO:O	2.03	0.59
1:F:256:ARG:HG2	1:F:263:PRO:HD3	1.84	0.59
1:D:226:VAL:CG2	1:D:280:LEU:HD23	2.31	0.59
1:D:272:ILE:HG12	1:D:273:ILE:N	2.17	0.58
1:G:197:VAL:HG21	1:G:208:THR:HG22	1.85	0.58
1:F:27:HIS:CD2	1:F:254:LEU:HD21	2.38	0.58
1:G:79:GLU:OE2	1:G:121:SER:HB2	2.04	0.58
1:C:93:ARG:HD3	1:D:132:TYR:OH	2.04	0.58
1:G:197:VAL:HG21	1:G:208:THR:CG2	2.33	0.58
1:A:243:VAL:HG11	1:A:294:LEU:HD13	1.84	0.58
1:C:110:SER:HB2	1:C:129:THR:HG23	1.85	0.58
1:G:162:ILE:HD11	1:G:239:VAL:CG2	2.34	0.58
1:A:164:GLN:HA	1:A:265:LEU:O	2.04	0.58
1:C:264:ILE:HB	1:C:276:VAL:HG22	1.85	0.58
1:A:191:LEU:HD12	1:A:198:THR:HG22	1.85	0.58
1:F:167:LEU:O	1:F:262:VAL:HG22	2.04	0.58
1:H:8:ARG:HG2	1:H:108:GLN:NE2	2.19	0.58
1:D:187:VAL:HG23	1:D:245:ALA:HB2	1.85	0.58
1:E:182:GLN:HA	1:E:182:GLN:HE21	1.68	0.58
1:D:197:VAL:HG11	1:D:208:THR:HG23	1.86	0.57
1:F:4:THR:OG1	1:F:5:GLN:NE2	2.37	0.57
1:H:171:THR:HG23	1:H:209:LEU:HD22	1.85	0.57
1:B:81:PRO:HA	1:G:230:GLN:NE2	2.19	0.57
1:C:12:LYS:HD3	1:C:106:VAL:O	2.03	0.57
1:C:128:LEU:HD12	1:C:128:LEU:H	1.68	0.57
1:G:39:SER:HA	1:G:42:TYR:CE2	2.38	0.57
1:B:191:LEU:CD2	1:B:235:VAL:HG13	2.29	0.57
1:C:23:HIS:CD2	1:C:257:ILE:HG12	2.38	0.57
1:H:162:ILE:CD1	1:H:239:VAL:HG11	2.35	0.57
1:A:94:THR:HG21	1:B:99:LYS:CE	2.35	0.57
1:A:81:PRO:HB3	1:A:122:ARG:HG2	1.85	0.57
1:E:81:PRO:HG3	1:E:122:ARG:HG2	1.86	0.57
1:B:131:GLU:HG2	1:B:138:LYS:HG2	1.85	0.57
1:B:130:MSE:HE3	1:B:141:HIS:HD2	1.69	0.56
1:B:80:ALA:O	1:G:212:LYS:NZ	2.39	0.56
1:D:129:THR:N	1:D:130:MSE:HE3	2.20	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:GLU:O	1:E:114:TYR:HB2	2.06	0.56
1:B:81:PRO:HA	1:G:230:GLN:HE22	1.70	0.56
1:F:122:ARG:NH2	2:F:503:CL:CL	2.75	0.56
1:B:36:ASN:HD22	1:B:151:PRO:HB3	1.70	0.56
1:B:45:PRO:HG2	1:B:71:TRP:CD2	2.40	0.56
1:C:175:LEU:HB3	1:C:252:LEU:HD13	1.87	0.56
1:G:182:GLN:HG2	1:G:202:SER:CB	2.36	0.56
1:C:197:VAL:HG21	1:C:208:THR:HG22	1.88	0.56
1:D:128:LEU:HB3	1:D:130:MSE:CE	2.34	0.56
1:E:12:LYS:HG2	1:E:107:GLU:HA	1.88	0.56
1:A:46:ARG:HE	1:A:62:GLU:CD	2.09	0.56
1:C:159:GLU:HB3	1:C:268:TYR:CD2	2.41	0.56
1:E:206:CYS:SG	1:E:207:LEU:N	2.78	0.56
1:G:213:PRO:O	1:G:214:LEU:HD23	2.04	0.56
1:G:156:LEU:O	1:G:159:GLU:HB2	2.05	0.56
1:C:34:GLN:HB2	1:C:84:VAL:O	2.06	0.55
1:D:230:GLN:HG2	1:D:232:VAL:HG23	1.87	0.55
1:E:115:LYS:HG2	1:E:116:ARG:H	1.70	0.55
1:G:175:LEU:HD13	1:G:252:LEU:HD11	1.87	0.55
1:A:177:LYS:HE2	1:A:181:GLN:HE22	1.71	0.55
1:E:23:HIS:HD2	1:E:257:ILE:HG12	1.71	0.55
1:H:177:LYS:O	1:H:181:GLN:HG3	2.06	0.55
1:C:154:ASP:OD1	1:C:157:ARG:HD2	2.06	0.55
1:F:187:VAL:HA	1:F:201:THR:O	2.07	0.55
1:H:1:MSE:CE	1:H:116:ARG:HA	2.37	0.55
1:E:37:LEU:O	1:E:40:VAL:HG23	2.07	0.55
1:E:193:PRO:HD2	1:E:238:HIS:CE1	2.41	0.55
1:A:196:TYR:HD2	1:A:213:PRO:HG3	1.69	0.55
1:D:160:GLN:OE1	1:D:269:ARG:HD2	2.07	0.55
1:G:139:SER:HB3	1:H:93:ARG:NH2	2.21	0.55
1:A:8:ARG:NH1	1:A:70:GLU:HB3	2.22	0.55
1:G:91:TYR:O	1:G:93:ARG:HG3	2.07	0.55
1:G:118:GLN:CD	1:G:118:GLN:H	2.10	0.55
1:D:161:MSE:HE1	1:D:266:ARG:CD	2.35	0.55
1:D:166:LEU:HD21	1:D:262:VAL:HG11	1.88	0.55
1:E:115:LYS:NZ	1:E:115:LYS:HB3	2.22	0.55
1:E:36:ASN:ND2	1:E:151:PRO:CB	2.70	0.55
1:C:243:VAL:HG12	1:C:244:ALA:N	2.22	0.55
1:B:214:LEU:HG	1:B:232:VAL:HG13	1.89	0.54
1:A:91:TYR:O	1:A:93:ARG:N	2.41	0.54
1:A:216:VAL:CG1	1:A:220:GLU:HB2	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:GLY:HA2	1:E:293:ILE:O	2.08	0.54
1:E:1:MSE:CE	1:E:116:ARG:HG2	2.37	0.54
1:F:36:ASN:HB3	1:F:46:ARG:HB2	1.90	0.54
1:F:115:LYS:HB3	1:F:123:PRO:HA	1.88	0.54
1:G:95:CYS:HA	1:H:95:CYS:SG	2.47	0.54
1:A:13:ALA:O	1:A:16:VAL:HG22	2.07	0.54
1:B:175:LEU:HD13	1:B:252:LEU:CD1	2.35	0.54
1:A:17:LEU:HD21	1:A:287:PRO:HD2	1.90	0.54
1:E:1:MSE:HG3	1:E:2:GLU:H	1.73	0.54
1:C:162:ILE:HD11	1:C:269:ARG:CG	2.37	0.54
1:D:37:LEU:O	1:D:40:VAL:HG23	2.08	0.54
1:D:134:ASP:C	1:D:136:VAL:H	2.12	0.54
1:E:1:MSE:HA	1:E:1:MSE:CE	2.37	0.54
1:E:81:PRO:HG3	1:E:122:ARG:HB3	1.90	0.54
1:A:53:ALA:HB2	1:A:59:ILE:HD11	1.91	0.54
1:A:188:LYS:HE3	1:A:240:VAL:HG11	1.88	0.54
1:G:162:ILE:HD11	1:G:239:VAL:CG1	2.38	0.54
1:H:5:GLN:NE2	1:H:123:PRO:HG2	2.23	0.54
1:D:37:LEU:HB2	1:D:82:ALA:O	2.07	0.53
1:G:114:TYR:CE1	1:G:125:PHE:HB2	2.43	0.53
1:F:87:ARG:HD2	3:F:509:HOH:O	2.09	0.53
1:E:91:TYR:O	1:E:93:ARG:HD3	2.08	0.53
1:G:157:ARG:O	1:G:158:ASN:HB2	2.08	0.53
1:B:196:TYR:CD2	1:B:213:PRO:CG	2.92	0.53
1:E:193:PRO:HD2	1:E:238:HIS:ND1	2.23	0.53
1:F:90:ALA:HB3	1:F:93:ARG:HB2	1.90	0.53
1:G:193:PRO:HG3	1:G:235:VAL:CG1	2.38	0.53
1:F:91:TYR:O	1:F:93:ARG:N	2.34	0.53
1:A:4:THR:OG1	1:A:123:PRO:HG3	2.09	0.53
1:E:37:LEU:HD13	1:E:83:ALA:HA	1.90	0.53
1:F:56:ALA:HB1	1:F:295:PHE:HB2	1.90	0.53
1:C:91:TYR:O	1:C:93:ARG:HG2	2.08	0.53
1:G:226:VAL:CG1	1:G:227:ALA:N	2.71	0.53
1:G:91:TYR:C	1:G:93:ARG:H	2.10	0.53
1:H:4:THR:HG21	1:H:123:PRO:HG3	1.90	0.53
1:B:163:GLY:HA2	1:B:218:PRO:HG3	1.91	0.53
1:D:182:GLN:HA	1:D:182:GLN:NE2	2.24	0.53
1:B:151:PRO:HB2	1:B:154:ASP:HB2	1.91	0.52
1:A:197:VAL:HG21	1:A:208:THR:HG22	1.91	0.52
1:C:178:TRP:O	1:C:182:GLN:HG2	2.08	0.52
1:D:226:VAL:HG22	1:D:279:LEU:C	2.30	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LYS:HB2	1:E:232:VAL:HG12	1.92	0.52
1:E:216:VAL:O	1:E:234:ALA:HB1	2.09	0.52
1:B:128:LEU:N	1:B:128:LEU:HD12	2.25	0.52
1:B:166:LEU:CD1	1:B:264:ILE:HG12	2.40	0.52
1:D:159:GLU:OE1	1:D:270:SER:HB2	2.10	0.52
1:E:11:THR:HG22	1:E:12:LYS:HG3	1.92	0.52
1:D:27:HIS:CD2	1:D:254:LEU:HD21	2.45	0.52
1:F:1:MSE:HE1	1:F:116:ARG:HG2	1.92	0.52
1:H:123:PRO:HB2	1:H:148:TYR:OH	2.09	0.52
1:H:128:LEU:HD12	1:H:128:LEU:N	2.22	0.52
1:B:216:VAL:CG1	1:B:220:GLU:HB2	2.40	0.52
1:B:34:GLN:HG3	1:B:85:SER:HB3	1.91	0.52
1:F:90:ALA:HB1	1:F:93:ARG:HH11	1.74	0.52
1:F:175:LEU:HG	1:F:209:LEU:HD11	1.92	0.52
1:H:32:VAL:CG1	1:H:146:MSE:HE1	2.40	0.51
1:B:214:LEU:O	1:B:216:VAL:N	2.40	0.51
1:F:96:VAL:CG2	1:F:99:LYS:HB2	2.38	0.51
1:H:100:GLU:CB	1:H:130:MSE:HE2	2.41	0.51
1:B:268:TYR:HB2	1:B:272:ILE:CG2	2.40	0.51
1:D:216:VAL:HB	1:D:220:GLU:HB2	1.93	0.51
1:E:4:THR:HG23	1:E:114:TYR:HA	1.92	0.51
1:B:198:THR:HG23	1:B:200:TYR:CE1	2.46	0.51
1:C:66:ASP:OD2	1:C:66:ASP:N	2.44	0.51
1:C:94:THR:HG21	1:D:99:LYS:HD2	1.93	0.51
1:G:6:THR:O	1:G:71:TRP:HA	2.09	0.51
1:G:192:ASN:OD1	1:G:194:ASP:HB2	2.10	0.51
1:H:198:THR:HG23	1:H:200:TYR:HE1	1.75	0.51
1:D:138:LYS:HE2	1:D:140:HIS:HE1	1.73	0.51
1:D:175:LEU:HD13	1:D:252:LEU:HD11	1.92	0.51
1:H:297:HIS:C	1:H:297:HIS:CD2	2.84	0.51
1:B:156:LEU:HD23	1:B:159:GLU:HG3	1.93	0.51
1:D:12:LYS:HZ3	1:D:105:ALA:C	2.13	0.51
1:A:128:LEU:N	1:A:128:LEU:HD12	2.26	0.51
1:E:133:ASP:O	1:E:135:LYS:N	2.43	0.51
1:F:48:ALA:CB	1:F:62:GLU:HB3	2.39	0.51
1:F:90:ALA:HB1	1:F:93:ARG:NH1	2.25	0.51
1:B:283:ALA:O	1:B:284:GLY:O	2.29	0.51
1:F:76:SER:OG	1:F:79:GLU:HG3	2.10	0.51
1:F:175:LEU:HD13	1:F:252:LEU:CD1	2.33	0.51
1:G:93:ARG:HH21	1:H:137:SER:HB3	1.76	0.51
1:H:155:ARG:HH22	1:H:272:ILE:HD11	1.73	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:O	1:B:239:VAL:HB	2.12	0.50
1:C:146:MSE:C	1:C:147:PRO:O	2.47	0.50
1:H:134:ASP:O	1:H:135:LYS:HB2	2.11	0.50
1:B:128:LEU:HD12	1:B:128:LEU:H	1.77	0.50
1:C:122:ARG:CG	1:C:148:TYR:OH	2.57	0.50
1:D:53:ALA:HB2	1:D:59:ILE:CD1	2.40	0.50
1:D:226:VAL:HG23	1:D:280:LEU:HA	1.94	0.50
1:F:7:LEU:HD13	1:F:71:TRP:HE3	1.76	0.50
1:H:199:THR:HG22	3:H:507:HOH:O	2.10	0.50
1:H:216:VAL:HB	1:H:220:GLU:CB	2.37	0.50
1:C:243:VAL:HG13	3:C:508:HOH:O	2.12	0.50
1:F:90:ALA:CB	1:F:93:ARG:HD2	2.41	0.50
1:H:13:ALA:O	1:H:16:VAL:HG22	2.12	0.50
1:H:214:LEU:HB2	1:H:233:GLY:O	2.12	0.50
1:B:118:GLN:O	1:B:119:GLY:C	2.49	0.50
1:E:1:MSE:CG	1:E:2:GLU:H	2.24	0.50
1:A:91:TYR:C	1:A:93:ARG:N	2.65	0.50
1:B:282:SER:O	1:B:283:ALA:C	2.50	0.50
1:C:58:LEU:HD21	1:C:152:ALA:HB1	1.93	0.50
1:D:45:PRO:HG2	1:D:71:TRP:CG	2.46	0.50
1:D:49:ALA:HB3	1:D:61:PHE:HB3	1.94	0.50
1:D:198:THR:HG22	1:D:200:TYR:CE1	2.47	0.50
1:E:83:ALA:CB	1:E:151:PRO:HG3	2.40	0.50
1:F:45:PRO:HG2	1:F:71:TRP:HB2	1.93	0.50
1:F:47:LEU:C	1:F:47:LEU:HD23	2.33	0.50
1:H:138:LYS:HE2	1:H:140:HIS:NE2	2.27	0.50
1:H:166:LEU:HD13	1:H:264:ILE:HG12	1.93	0.50
1:A:70:GLU:OE1	1:A:72:GLN:NE2	2.45	0.50
1:B:193:PRO:HD2	1:B:238:HIS:CD2	2.47	0.50
1:E:38:LEU:HD12	1:E:38:LEU:H	1.77	0.50
1:G:93:ARG:NH1	1:G:141:HIS:ND1	2.60	0.50
1:B:190:THR:HB	1:B:199:THR:OG1	2.12	0.49
1:G:164:GLN:HA	1:G:265:LEU:O	2.12	0.49
1:A:243:VAL:HG12	1:A:244:ALA:N	2.27	0.49
1:G:36:ASN:HD21	1:G:38:LEU:H	1.58	0.49
1:G:99:LYS:HG3	1:H:94:THR:HG21	1.93	0.49
1:C:200:TYR:CD1	1:C:200:TYR:N	2.81	0.49
1:D:10:LYS:HB2	1:D:13:ALA:HB2	1.94	0.49
1:G:191:LEU:HD21	1:G:235:VAL:HG13	1.94	0.49
1:B:57:GLY:HA2	1:B:293:ILE:O	2.12	0.49
1:D:180:ARG:HH11	1:D:180:ARG:HG2	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLY:HA3	1:G:51:ALA:HB2	1.93	0.49
1:F:5:GLN:NE2	1:F:123:PRO:HG2	2.27	0.49
1:F:86:PHE:HA	1:F:146:MSE:HG3	1.93	0.49
1:A:191:LEU:HD21	1:A:235:VAL:HG13	1.95	0.49
1:A:230:GLN:HG3	1:A:232:VAL:HG13	1.93	0.49
1:F:134:ASP:O	1:F:136:VAL:HG23	2.13	0.49
1:G:39:SER:O	1:G:41:ASN:N	2.45	0.49
1:A:100:GLU:HB3	1:A:130:MSE:CE	2.40	0.49
1:B:282:SER:O	1:B:284:GLY:N	2.46	0.49
1:C:197:VAL:HG21	1:C:208:THR:CG2	2.43	0.49
1:E:192:ASN:O	1:E:195:LEU:O	2.31	0.49
1:B:207:LEU:HD11	1:B:209:LEU:HD21	1.95	0.49
1:E:239:VAL:HG12	1:E:240:VAL:N	2.28	0.49
1:F:46:ARG:HD3	1:F:62:GLU:OE1	2.13	0.49
1:F:63:VAL:HA	1:F:287:PRO:O	2.13	0.49
1:G:214:LEU:HD11	1:G:232:VAL:HG11	1.95	0.49
1:A:8:ARG:NH1	1:A:70:GLU:OE2	2.40	0.49
1:A:90:ALA:HB2	1:A:97:LEU:HD21	1.94	0.49
1:B:37:LEU:HD13	1:B:83:ALA:HA	1.95	0.49
1:E:286:LEU:HD12	1:E:286:LEU:N	2.27	0.49
1:F:9:PHE:O	1:F:108:GLN:NE2	2.46	0.49
1:H:9:PHE:CE2	1:H:68:VAL:HG22	2.48	0.49
1:A:37:LEU:O	1:A:40:VAL:HG23	2.12	0.48
1:E:243:VAL:HG11	1:E:294:LEU:HD13	1.94	0.48
1:H:42:TYR:HD1	1:H:42:TYR:O	1.96	0.48
1:E:126:VAL:O	1:E:142:THR:HA	2.14	0.48
1:E:214:LEU:HD22	1:E:216:VAL:CG1	2.43	0.48
1:C:176:GLN:OE1	1:C:253:SER:HB2	2.12	0.48
1:E:32:VAL:HG11	1:E:146:MSE:HE1	1.94	0.48
1:H:112:GLN:NE2	1:H:114:TYR:CE2	2.80	0.48
1:B:36:ASN:ND2	1:B:151:PRO:CB	2.76	0.48
1:D:12:LYS:HE2	1:D:107:GLU:HG3	1.95	0.48
1:G:187:VAL:HG23	1:G:245:ALA:HB2	1.94	0.48
1:G:227:ALA:C	1:G:229:ALA:H	2.16	0.48
1:B:91:TYR:O	1:B:93:ARG:N	2.44	0.48
1:C:86:PHE:HA	1:C:146:MSE:CG	2.39	0.48
1:F:12:LYS:O	1:F:16:VAL:HG23	2.13	0.48
1:F:133:ASP:C	1:F:135:LYS:H	2.16	0.48
1:C:1:MSE:HB3	1:C:117:PRO:HD3	1.95	0.48
1:F:48:ALA:HB2	1:F:62:GLU:CB	2.42	0.48
1:B:46:ARG:HD3	1:B:62:GLU:OE2	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ALA:O	1:D:16:VAL:HG22	2.13	0.48
1:E:1:MSE:HE1	1:E:116:ARG:HG2	1.95	0.48
1:H:221:ALA:O	1:H:222:PHE:C	2.51	0.48
1:A:168:MSE:HG2	1:A:231:ASP:OD1	2.13	0.48
1:F:93:ARG:HH11	1:F:93:ARG:HG3	1.79	0.48
1:G:90:ALA:HB3	1:G:93:ARG:HD2	1.95	0.48
1:A:216:VAL:HG12	1:A:217:GLY:N	2.28	0.48
1:B:10:LYS:HE3	1:B:68:VAL:O	2.14	0.48
1:F:73:ASN:HD22	1:F:74:HIS:N	2.11	0.48
1:B:268:TYR:O	1:B:270:SER:O	2.32	0.48
1:E:290:LEU:HD12	1:E:291:SER:N	2.29	0.48
1:B:39:SER:HA	1:B:42:TYR:HD1	1.79	0.47
1:C:17:LEU:HD21	1:C:287:PRO:HD2	1.95	0.47
1:C:243:VAL:CG1	1:C:244:ALA:N	2.76	0.47
1:E:100:GLU:HB2	1:E:130:MSE:HE2	1.95	0.47
1:G:22:ASP:OD1	1:G:99:LYS:NZ	2.39	0.47
1:G:151:PRO:HB2	1:G:154:ASP:OD2	2.14	0.47
1:A:110:SER:C	1:A:111:LEU:HD12	2.35	0.47
1:A:127:LYS:HA	1:A:141:HIS:O	2.15	0.47
1:B:129:THR:HA	1:B:130:MSE:HE2	1.95	0.47
1:D:1:MSE:HA	1:D:117:PRO:CD	2.43	0.47
1:D:207:LEU:HD23	1:D:208:THR:N	2.29	0.47
1:E:85:SER:OG	1:E:149:MSE:HE3	2.14	0.47
1:C:129:THR:N	1:C:130:MSE:HE2	2.29	0.47
1:D:265:LEU:HD22	1:D:275:VAL:HG22	1.97	0.47
1:D:270:SER:CB	1:D:272:ILE:HG22	2.36	0.47
1:E:207:LEU:HD11	1:E:209:LEU:HD21	1.95	0.47
1:H:17:LEU:HD22	1:H:288:LEU:HB2	1.96	0.47
1:A:111:LEU:HD12	1:A:111:LEU:N	2.29	0.47
1:B:17:LEU:HD21	1:B:287:PRO:HD2	1.95	0.47
1:E:1:MSE:HG3	1:E:2:GLU:N	2.30	0.47
1:E:164:GLN:NE2	1:E:218:PRO:O	2.45	0.47
1:E:216:VAL:CG2	1:E:220:GLU:HB2	2.43	0.47
1:B:118:GLN:O	1:B:119:GLY:O	2.32	0.47
1:E:166:LEU:HD21	1:E:262:VAL:CG1	2.44	0.47
1:E:191:LEU:HD21	1:E:235:VAL:HG13	1.97	0.47
1:E:197:VAL:HG12	1:E:210:ASP:OD1	2.14	0.47
1:E:243:VAL:CG1	1:E:244:ALA:N	2.77	0.47
1:G:94:THR:HB	1:H:100:GLU:OE2	2.15	0.47
1:H:169:PRO:HD3	1:H:229:ALA:HB1	1.96	0.47
1:D:214:LEU:HD21	1:D:232:VAL:HG11	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLU:CG	1:E:138:LYS:HE2	2.42	0.47
1:E:175:LEU:HB3	1:E:252:LEU:CD1	2.44	0.47
1:E:246:ASP:OD2	1:E:247:SER:N	2.47	0.47
1:F:112:GLN:O	1:F:126:VAL:HA	2.15	0.47
1:A:235:VAL:HG12	1:A:236:GLU:H	1.77	0.47
1:D:281:THR:O	1:D:283:ALA:O	2.33	0.47
1:A:133:ASP:HB2	1:B:91:TYR:OH	2.14	0.47
1:A:190:THR:HB	1:A:199:THR:OG1	2.15	0.47
1:C:37:LEU:HD12	1:C:81:PRO:HG2	1.97	0.47
1:C:243:VAL:HG13	1:C:294:LEU:HB3	1.97	0.47
1:E:115:LYS:HG2	1:E:116:ARG:N	2.29	0.47
1:H:50:VAL:HA	1:H:59:ILE:O	2.15	0.47
1:H:191:LEU:HD11	1:H:267:PHE:CG	2.50	0.47
1:B:122:ARG:NH2	1:G:230:GLN:HG2	2.30	0.46
1:B:164:GLN:HA	1:B:265:LEU:O	2.15	0.46
1:F:44:GLY:H	1:F:65:PRO:HG2	1.80	0.46
1:G:173:SER:HB3	1:G:256:ARG:HH12	1.80	0.46
1:C:65:PRO:C	1:C:67:ALA:H	2.18	0.46
1:H:95:CYS:SG	1:H:100:GLU:OE2	2.73	0.46
1:A:235:VAL:CG1	1:A:236:GLU:N	2.76	0.46
1:B:12:LYS:HE2	1:B:133:ASP:OD1	2.16	0.46
1:F:91:TYR:C	1:F:93:ARG:H	2.15	0.46
1:G:214:LEU:HG	1:G:232:VAL:HG13	1.98	0.46
1:E:9:PHE:CD2	1:E:14:LEU:HD21	2.50	0.46
1:F:66:ASP:OD2	1:F:66:ASP:N	2.48	0.46
1:H:42:TYR:O	1:H:42:TYR:CD1	2.68	0.46
1:E:36:ASN:ND2	1:E:151:PRO:HB3	2.30	0.46
1:F:83:ALA:CB	1:F:151:PRO:HG3	2.43	0.46
1:G:95:CYS:SG	1:G:100:GLU:HG3	2.55	0.46
1:H:46:ARG:HD2	3:H:505:HOH:O	2.15	0.46
1:H:201:THR:HG22	1:H:206:CYS:CB	2.42	0.46
1:A:243:VAL:CG1	1:A:244:ALA:N	2.78	0.46
1:B:6:THR:HB	1:B:72:GLN:HB2	1.97	0.46
1:H:37:LEU:O	1:H:40:VAL:HG23	2.15	0.46
1:B:216:VAL:HG12	1:B:217:GLY:N	2.30	0.46
1:D:147:PRO:O	1:D:148:TYR:C	2.50	0.46
1:F:1:MSE:CE	1:F:116:ARG:HA	2.46	0.46
1:B:37:LEU:HD12	1:B:37:LEU:N	2.31	0.46
1:C:5:GLN:HE21	1:C:5:GLN:HB3	1.56	0.46
1:C:22:ASP:O	1:C:25:GLN:HG2	2.16	0.46
1:C:91:TYR:OH	1:D:133:ASP:HB2	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:LEU:HD12	1:G:264:ILE:HG12	1.97	0.46
1:A:118:GLN:O	1:A:119:GLY:C	2.54	0.46
1:A:286:LEU:HA	1:A:287:PRO:HD3	1.82	0.46
1:B:115:LYS:HG2	1:B:116:ARG:N	2.31	0.46
1:C:100:GLU:OE1	1:D:95:CYS:SG	2.74	0.46
1:D:214:LEU:HD21	1:D:232:VAL:CG1	2.46	0.46
1:F:116:ARG:HG3	1:F:124:GLU:OE1	2.16	0.46
1:G:45:PRO:HG2	1:G:71:TRP:CG	2.51	0.46
1:C:65:PRO:C	1:C:67:ALA:N	2.69	0.46
1:E:5:GLN:NE2	1:E:73:ASN:OD1	2.35	0.46
1:B:260:VAL:HA	1:B:283:ALA:HB2	1.98	0.45
1:D:4:THR:HG21	1:D:123:PRO:HG3	1.98	0.45
1:E:4:THR:HG21	1:E:123:PRO:HG3	1.98	0.45
1:G:33:LEU:HD23	1:G:33:LEU:HA	1.85	0.45
1:C:149:MSE:HA	1:C:150:PRO:HD2	1.61	0.45
1:C:197:VAL:CG2	1:C:208:THR:HG22	2.46	0.45
1:F:47:LEU:HD23	1:F:48:ALA:N	2.30	0.45
1:G:36:ASN:HD21	1:G:38:LEU:HB2	1.81	0.45
1:G:53:ALA:HB2	1:G:59:ILE:CG1	2.46	0.45
1:B:118:GLN:H	1:B:118:GLN:HG2	1.39	0.45
1:B:230:GLN:HG3	1:B:232:VAL:HG23	1.98	0.45
1:C:2:GLU:HG2	1:C:117:PRO:HG3	1.99	0.45
1:D:122:ARG:NH1	1:D:148:TYR:CD2	2.77	0.45
1:E:35:VAL:HB	1:E:84:VAL:HG23	1.97	0.45
1:H:262:VAL:HG13	1:H:280:LEU:HD21	1.97	0.45
1:A:9:PHE:CE2	1:A:68:VAL:HG22	2.52	0.45
1:E:46:ARG:HD3	1:E:62:GLU:OE1	2.15	0.45
1:E:290:LEU:HD12	1:E:291:SER:H	1.81	0.45
1:E:10:LYS:HE3	1:E:68:VAL:O	2.17	0.45
1:E:200:TYR:CD1	1:E:200:TYR:N	2.84	0.45
1:F:197:VAL:HG12	1:F:210:ASP:OD1	2.16	0.45
1:H:138:LYS:HE2	1:H:140:HIS:CE1	2.51	0.45
1:A:197:VAL:HG21	1:A:208:THR:CG2	2.47	0.45
1:H:176:GLN:OE1	1:H:253:SER:HB2	2.17	0.45
1:B:86:PHE:N	1:B:86:PHE:CD2	2.84	0.45
1:E:191:LEU:HD11	1:E:235:VAL:HG21	1.99	0.45
1:H:47:LEU:HD21	1:H:101:LEU:HD11	1.98	0.45
1:A:93:ARG:HH21	1:B:137:SER:HB3	1.79	0.45
1:A:226:VAL:HG22	1:A:279:LEU:O	2.17	0.45
1:C:122:ARG:HG3	1:C:148:TYR:CZ	2.51	0.45
1:C:198:THR:HG21	1:C:200:TYR:OH	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ALA:O	1:E:16:VAL:HG22	2.17	0.45
1:E:166:LEU:HD23	1:E:167:LEU:H	1.82	0.45
1:F:12:LYS:HD3	1:F:106:VAL:O	2.16	0.45
1:G:177:LYS:O	1:G:181:GLN:HG3	2.16	0.45
1:A:133:ASP:C	1:A:135:LYS:H	2.20	0.45
1:B:268:TYR:HB2	1:B:272:ILE:HG22	1.99	0.45
1:C:25:GLN:NE2	1:C:99:LYS:HE3	2.31	0.45
1:C:93:ARG:HH11	1:C:93:ARG:CG	2.29	0.45
1:C:148:TYR:N	1:C:148:TYR:CD1	2.83	0.45
1:C:243:VAL:CG1	1:C:294:LEU:HB3	2.45	0.45
1:E:2:GLU:HB3	1:E:115:LYS:O	2.16	0.45
1:A:27:HIS:ND1	1:A:254:LEU:HD21	2.32	0.45
1:B:156:LEU:CD2	1:B:159:GLU:HG3	2.47	0.45
1:C:1:MSE:HE2	1:C:117:PRO:HD2	1.99	0.45
1:E:3:THR:HA	1:E:114:TYR:HB3	1.99	0.44
1:F:73:ASN:HD22	1:F:73:ASN:C	2.20	0.44
1:A:122:ARG:NH2	1:A:148:TYR:HB2	2.31	0.44
1:A:146:MSE:HB3	1:A:147:PRO:HD2	1.99	0.44
1:D:129:THR:CA	1:D:130:MSE:HE3	2.47	0.44
1:D:146:MSE:O	1:D:147:PRO:C	2.54	0.44
1:D:197:VAL:CG1	1:D:208:THR:HG23	2.46	0.44
1:E:165:VAL:HG13	1:E:267:PHE:HE1	1.81	0.44
1:F:115:LYS:HD2	1:F:120:GLY:O	2.17	0.44
1:G:230:GLN:HB2	1:G:232:VAL:HG23	1.98	0.44
1:H:7:LEU:CD1	1:H:71:TRP:HE3	2.26	0.44
1:A:200:TYR:N	1:A:200:TYR:CD1	2.86	0.44
1:C:175:LEU:HD11	1:C:200:TYR:CE2	2.52	0.44
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.87	0.44
1:D:150:PRO:O	1:D:151:PRO:C	2.54	0.44
1:E:101:LEU:HD13	1:E:101:LEU:O	2.17	0.44
1:F:8:ARG:NH1	1:F:70:GLU:HB3	2.33	0.44
1:F:25:GLN:HG3	3:F:513:HOH:O	2.17	0.44
1:B:168:MSE:CE	1:B:230:GLN:HA	2.47	0.44
1:D:149:MSE:HE2	1:D:149:MSE:HB2	1.76	0.44
1:F:9:PHE:CE2	1:F:68:VAL:HG22	2.52	0.44
1:F:162:ILE:CD1	1:F:239:VAL:HG11	2.48	0.44
1:F:178:TRP:O	1:F:182:GLN:HG2	2.17	0.44
1:G:64:SER:OG	1:G:66:ASP:OD1	2.34	0.44
1:G:178:TRP:O	1:G:182:GLN:NE2	2.50	0.44
1:B:70:GLU:HG2	1:B:72:GLN:HE21	1.82	0.44
1:B:78:GLU:H	1:B:78:GLU:HG2	1.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:THR:HG23	1:B:240:VAL:HG22	1.99	0.44
1:C:37:LEU:CD2	1:C:71:TRP:CZ2	3.01	0.44
1:C:155:ARG:NE	1:C:155:ARG:HA	2.32	0.44
1:C:166:LEU:HD23	1:C:166:LEU:C	2.38	0.44
1:H:115:LYS:HD2	1:H:120:GLY:C	2.38	0.44
1:B:90:ALA:HB3	1:B:93:ARG:CG	2.42	0.44
1:E:133:ASP:C	1:E:135:LYS:H	2.21	0.44
1:C:115:LYS:HD2	1:C:120:GLY:O	2.18	0.44
1:F:133:ASP:O	1:F:135:LYS:N	2.51	0.44
1:B:87:ARG:HG3	1:B:89:LEU:O	2.18	0.43
1:C:53:ALA:HB2	1:C:59:ILE:HG13	1.99	0.43
1:D:163:GLY:HA2	1:D:218:PRO:HG3	2.00	0.43
1:E:32:VAL:CG2	1:E:50:VAL:HG22	2.48	0.43
1:E:36:ASN:HD22	1:E:151:PRO:HB3	1.83	0.43
1:E:42:TYR:O	1:E:42:TYR:CD1	2.71	0.43
1:H:246:ASP:OD2	1:H:247:SER:N	2.51	0.43
1:A:45:PRO:HG2	1:A:71:TRP:CD2	2.53	0.43
1:D:111:LEU:CD2	1:D:128:LEU:HG	2.45	0.43
1:D:129:THR:N	1:D:130:MSE:CE	2.81	0.43
1:G:8:ARG:HG3	1:G:108:GLN:HE22	1.83	0.43
1:G:197:VAL:HG23	1:G:209:LEU:C	2.38	0.43
1:H:5:GLN:HE22	1:H:123:PRO:HG2	1.83	0.43
1:A:80:ALA:O	1:F:212:LYS:NZ	2.51	0.43
1:C:17:LEU:HD22	1:C:288:LEU:HB2	2.00	0.43
1:D:93:ARG:HG3	1:D:95:CYS:H	1.83	0.43
1:G:90:ALA:CB	1:G:93:ARG:HD2	2.48	0.43
1:G:227:ALA:O	1:G:229:ALA:N	2.51	0.43
1:H:195:LEU:O	1:H:196:TYR:HB2	2.19	0.43
1:A:64:SER:HB3	1:A:66:ASP:OD1	2.19	0.43
1:E:166:LEU:HB2	1:E:222:PHE:CE2	2.53	0.43
1:F:128:LEU:N	1:F:128:LEU:HD12	2.32	0.43
1:G:163:GLY:HA2	1:G:234:ALA:O	2.18	0.43
1:A:193:PRO:HG3	1:A:235:VAL:CG1	2.48	0.43
1:B:198:THR:CG2	1:B:209:LEU:HB2	2.47	0.43
1:F:1:MSE:HE1	1:F:116:ARG:HA	2.00	0.43
1:F:191:LEU:HD12	1:F:239:VAL:CG2	2.48	0.43
1:F:230:GLN:HG3	1:F:232:VAL:HG23	2.00	0.43
1:G:227:ALA:C	1:G:229:ALA:N	2.71	0.43
1:A:128:LEU:HD12	1:A:128:LEU:H	1.83	0.43
1:A:196:TYR:CD2	1:A:213:PRO:CG	3.00	0.43
1:B:155:ARG:CD	1:B:155:ARG:O	2.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ARG:HG2	1:D:157:ARG:HH11	1.82	0.43
1:D:226:VAL:CG2	1:D:280:LEU:HA	2.49	0.43
1:E:162:ILE:C	1:E:162:ILE:HD12	2.39	0.43
1:E:166:LEU:HD21	1:E:262:VAL:HG11	2.01	0.43
1:E:257:ILE:HB	1:E:260:VAL:HB	2.00	0.43
1:F:166:LEU:C	1:F:166:LEU:HD23	2.39	0.43
1:F:169:PRO:HD3	1:F:228:LYS:HB2	2.01	0.43
1:G:36:ASN:ND2	1:G:37:LEU:N	2.66	0.43
1:H:8:ARG:NH1	1:H:70:GLU:OE2	2.52	0.43
1:A:166:LEU:HD23	1:A:167:LEU:N	2.33	0.43
1:A:226:VAL:HG23	1:A:226:VAL:O	2.18	0.43
1:B:214:LEU:HG	1:B:232:VAL:CG1	2.49	0.43
1:C:166:LEU:HD21	1:C:262:VAL:HG11	2.01	0.43
1:E:48:ALA:HB2	1:E:62:GLU:HG2	2.00	0.43
1:H:146:MSE:HB3	1:H:147:PRO:CD	2.49	0.43
1:A:8:ARG:CD	1:A:108:GLN:OE1	2.66	0.43
1:B:33:LEU:HD12	1:B:86:PHE:CE1	2.53	0.43
1:E:42:TYR:O	1:E:42:TYR:HD1	2.01	0.43
1:E:100:GLU:CB	1:E:130:MSE:HE2	2.48	0.43
1:E:276:VAL:HG12	1:E:277:ALA:N	2.33	0.43
1:H:175:LEU:HD13	1:H:252:LEU:CD1	2.45	0.43
1:A:201:THR:HG22	1:A:206:CYS:HB2	2.01	0.43
1:D:175:LEU:HB3	1:D:252:LEU:HD13	1.99	0.43
1:H:216:VAL:HG12	1:H:220:GLU:OE1	2.19	0.43
1:H:281:THR:O	1:H:283:ALA:O	2.37	0.43
1:H:286:LEU:C	1:H:288:LEU:H	2.22	0.43
1:A:39:SER:OG	1:A:46:ARG:HG3	2.18	0.43
1:B:191:LEU:HD11	1:B:235:VAL:HG21	2.00	0.43
1:D:127:LYS:HA	1:D:141:HIS:O	2.19	0.43
1:E:32:VAL:HG22	1:E:50:VAL:HG22	2.01	0.43
1:E:214:LEU:HD22	1:E:216:VAL:HG12	2.01	0.43
1:H:161:MSE:HE3	1:H:218:PRO:C	2.39	0.43
1:A:64:SER:CB	1:A:66:ASP:OD1	2.68	0.42
1:B:191:LEU:CD2	1:B:235:VAL:CG1	2.94	0.42
1:C:37:LEU:O	1:C:40:VAL:HG23	2.18	0.42
1:D:115:LYS:HB3	1:D:123:PRO:HA	2.00	0.42
1:D:146:MSE:C	1:D:147:PRO:O	2.56	0.42
1:E:22:ASP:HA	1:E:25:GLN:HE21	1.84	0.42
1:E:180:ARG:HG2	1:E:180:ARG:HH11	1.84	0.42
1:G:133:ASP:O	1:G:135:LYS:N	2.52	0.42
1:H:90:ALA:HB3	1:H:93:ARG:HB2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:GLU:OE1	1:D:270:SER:CB	2.67	0.42
1:D:197:VAL:CG1	1:D:198:THR:N	2.81	0.42
1:G:207:LEU:HD11	1:G:209:LEU:HD21	2.01	0.42
1:C:283:ALA:O	1:C:284:GLY:O	2.36	0.42
1:D:1:MSE:N	1:D:117:PRO:HG3	2.34	0.42
1:E:7:LEU:HD13	1:E:71:TRP:CE3	2.53	0.42
1:E:48:ALA:HA	1:E:61:PHE:O	2.19	0.42
1:F:93:ARG:NH1	1:F:93:ARG:HG3	2.34	0.42
1:F:133:ASP:C	1:F:135:LYS:N	2.72	0.42
1:G:146:MSE:HB3	1:G:147:PRO:CD	2.49	0.42
1:C:128:LEU:HD12	1:C:128:LEU:N	2.34	0.42
1:E:101:LEU:CA	1:E:130:MSE:HE3	2.49	0.42
1:G:87:ARG:HD2	3:G:510:HOH:O	2.18	0.42
1:C:116:ARG:O	1:C:117:PRO:C	2.58	0.42
1:E:151:PRO:O	1:E:152:ALA:C	2.57	0.42
1:G:8:ARG:CG	1:G:108:GLN:HE22	2.32	0.42
1:G:11:THR:O	1:G:12:LYS:HB2	2.20	0.42
1:G:36:ASN:ND2	1:G:36:ASN:C	2.73	0.42
1:H:200:TYR:N	1:H:200:TYR:CD1	2.88	0.42
1:A:112:GLN:HE21	1:A:112:GLN:HB3	1.60	0.42
1:F:21:TYR:O	1:F:25:GLN:N	2.44	0.42
1:G:166:LEU:HD11	1:G:226:VAL:HG11	2.01	0.42
1:C:196:TYR:CD2	1:C:196:TYR:N	2.85	0.42
1:E:166:LEU:HD23	1:E:167:LEU:N	2.34	0.42
1:E:182:GLN:NE2	1:E:182:GLN:CA	2.78	0.42
1:F:193:PRO:HD2	1:F:238:HIS:CE1	2.54	0.42
1:G:116:ARG:HB3	1:G:118:GLN:HE22	1.84	0.42
1:A:95:CYS:HB2	1:B:100:GLU:OE2	2.20	0.42
1:B:129:THR:HA	1:B:139:SER:O	2.20	0.42
1:E:32:VAL:CG1	1:E:146:MSE:HE1	2.50	0.42
1:E:169:PRO:HD3	1:E:229:ALA:HB3	2.00	0.42
1:F:189:VAL:CG1	1:F:267:PHE:HE2	2.32	0.42
1:G:66:ASP:OD1	1:G:66:ASP:N	2.53	0.42
1:G:200:TYR:O	1:G:206:CYS:HA	2.19	0.42
1:H:161:MSE:HE1	1:H:219:TYR:HA	2.02	0.42
1:H:196:TYR:CG	1:H:213:PRO:HG3	2.55	0.42
1:A:133:ASP:C	1:A:135:LYS:N	2.72	0.42
1:A:212:LYS:HA	1:A:213:PRO:HD3	1.78	0.42
1:D:81:PRO:HB2	1:D:148:TYR:HE2	1.84	0.42
1:E:221:ALA:HB1	1:E:222:PHE:CE1	2.55	0.42
1:B:268:TYR:HB2	1:B:272:ILE:HG23	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:SER:HA	1:F:65:PRO:HD3	1.92	0.42
1:G:13:ALA:O	1:G:16:VAL:HG22	2.20	0.42
1:H:166:LEU:HD12	1:H:167:LEU:N	2.35	0.42
1:H:198:THR:HG23	1:H:200:TYR:CE1	2.54	0.42
1:D:6:THR:O	1:D:71:TRP:HA	2.20	0.41
1:E:23:HIS:CD2	1:E:257:ILE:HG12	2.54	0.41
1:F:73:ASN:HD21	1:F:75:GLN:HB2	1.84	0.41
1:D:212:LYS:HA	1:D:213:PRO:HD3	1.93	0.41
1:E:197:VAL:CG1	1:E:210:ASP:OD1	2.68	0.41
1:F:146:MSE:HB3	1:F:147:PRO:HD2	2.01	0.41
1:C:53:ALA:HB2	1:C:59:ILE:CG1	2.51	0.41
1:E:214:LEU:O	1:E:216:VAL:N	2.54	0.41
1:G:94:THR:HG21	1:H:99:LYS:CE	2.49	0.41
1:H:83:ALA:HB2	1:H:151:PRO:HG3	2.02	0.41
1:H:146:MSE:HB3	1:H:147:PRO:HD2	2.01	0.41
1:B:208:THR:O	1:C:204:GLU:HB3	2.20	0.41
1:B:257:ILE:HD11	1:B:290:LEU:HD12	2.01	0.41
1:C:269:ARG:C	1:C:271:GLY:H	2.22	0.41
1:E:122:ARG:HB3	1:E:123:PRO:HD2	2.01	0.41
1:B:146:MSE:HB3	1:B:147:PRO:HD2	2.03	0.41
1:D:167:LEU:O	1:D:262:VAL:HG13	2.21	0.41
1:E:193:PRO:HG3	1:E:235:VAL:HG12	2.03	0.41
1:F:90:ALA:HB3	1:F:93:ARG:HD2	2.01	0.41
1:F:133:ASP:O	1:F:135:LYS:HG3	2.20	0.41
1:G:45:PRO:HG2	1:G:71:TRP:CD2	2.54	0.41
1:H:214:LEU:HG	1:H:232:VAL:CG1	2.51	0.41
1:A:108:GLN:HE21	1:A:108:GLN:HB2	1.51	0.41
1:D:180:ARG:HG2	1:D:180:ARG:NH1	2.35	0.41
1:E:14:LEU:HD13	1:E:101:LEU:CD1	2.51	0.41
1:E:122:ARG:HB3	1:E:123:PRO:CD	2.50	0.41
1:E:162:ILE:HD11	1:E:239:VAL:HG21	2.03	0.41
1:E:286:LEU:H	1:E:286:LEU:CD1	2.29	0.41
1:F:14:LEU:HD22	1:F:63:VAL:HG11	2.02	0.41
1:A:116:ARG:C	1:A:118:GLN:H	2.22	0.41
1:A:175:LEU:HD11	1:A:200:TYR:CE2	2.56	0.41
1:B:236:GLU:HG3	1:B:236:GLU:O	2.20	0.41
1:H:53:ALA:HB2	1:H:59:ILE:CG1	2.50	0.41
1:H:90:ALA:HB1	1:H:93:ARG:HD3	2.03	0.41
1:B:191:LEU:HB3	1:B:239:VAL:HG12	2.02	0.41
1:C:65:PRO:O	1:C:67:ALA:N	2.53	0.41
1:C:150:PRO:HA	1:C:151:PRO:HD3	1.92	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:GLN:O	1:C:232:VAL:HG23	2.20	0.41
1:D:168:MSE:HG2	1:D:230:GLN:N	2.32	0.41
1:E:34:GLN:CG	1:E:85:SER:HB3	2.42	0.41
1:G:2:GLU:O	1:G:114:TYR:HB2	2.20	0.41
1:A:112:GLN:NE2	1:A:114:TYR:OH	2.54	0.41
1:A:116:ARG:HA	1:A:117:PRO:HD3	1.94	0.41
1:A:197:VAL:CG2	1:A:208:THR:HG22	2.50	0.41
1:A:268:TYR:HB2	1:A:272:ILE:CG2	2.51	0.41
1:B:207:LEU:HD22	1:C:204:GLU:O	2.21	0.41
1:C:93:ARG:CG	1:C:93:ARG:NH1	2.84	0.41
1:C:113:PHE:CD1	1:C:113:PHE:N	2.89	0.41
1:C:140:HIS:O	1:D:139:SER:HA	2.21	0.41
1:C:154:ASP:OD2	1:C:157:ARG:NH1	2.54	0.41
1:E:166:LEU:HD12	1:E:222:PHE:CE2	2.55	0.41
1:E:197:VAL:HG12	1:E:210:ASP:HA	2.02	0.41
1:G:91:TYR:C	1:G:93:ARG:N	2.73	0.41
1:G:133:ASP:C	1:G:135:LYS:H	2.24	0.41
1:B:129:THR:CA	1:B:130:MSE:HE2	2.51	0.41
1:E:187:VAL:HA	1:E:201:THR:O	2.21	0.41
1:G:100:GLU:OE2	1:H:95:CYS:HB2	2.21	0.41
1:G:162:ILE:HD11	1:G:239:VAL:HG22	2.01	0.41
1:G:286:LEU:HA	1:G:287:PRO:HD3	1.79	0.41
1:A:31:GLY:HA3	1:A:51:ALA:HB2	2.04	0.40
1:A:40:VAL:HG22	1:A:45:PRO:HG3	2.02	0.40
1:B:7:LEU:HB2	1:B:71:TRP:CZ3	2.55	0.40
1:E:11:THR:HG23	1:E:107:GLU:HG3	2.03	0.40
1:F:146:MSE:O	1:F:147:PRO:C	2.60	0.40
1:A:45:PRO:CG	1:A:71:TRP:CD2	3.05	0.40
1:A:126:VAL:HG22	1:A:127:LYS:N	2.37	0.40
1:D:161:MSE:HE2	1:D:266:ARG:HD3	2.02	0.40
1:E:80:ALA:HA	1:E:81:PRO:HD3	1.93	0.40
1:E:243:VAL:HG12	1:E:244:ALA:O	2.21	0.40
1:G:200:TYR:CD1	1:G:200:TYR:N	2.89	0.40
1:G:246:ASP:OD2	1:G:247:SER:N	2.53	0.40
1:B:216:VAL:CG1	1:B:217:GLY:N	2.84	0.40
1:D:161:MSE:CE	1:D:266:ARG:CD	2.96	0.40
1:E:53:ALA:HB2	1:E:59:ILE:CG1	2.51	0.40
1:G:55:THR:HG23	1:G:246:ASP:OD1	2.20	0.40
1:G:95:CYS:CA	1:H:95:CYS:SG	3.09	0.40
1:C:122:ARG:HB2	1:C:123:PRO:HD2	2.04	0.40
1:D:214:LEU:HD11	1:D:232:VAL:CG1	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:VAL:HG23	1:G:209:LEU:O	2.21	0.40
1:G:229:ALA:C	1:G:230:GLN:HG3	2.41	0.40
1:B:171:THR:HG23	1:B:209:LEU:HD22	2.03	0.40
1:C:108:GLN:HB3	1:C:131:GLU:HB2	2.03	0.40
1:D:257:ILE:HB	1:D:260:VAL:HB	2.03	0.40
1:F:276:VAL:HG12	1:F:291:SER:HB3	2.02	0.40
1:G:100:GLU:HB3	3:G:511:HOH:O	2.21	0.40
1:G:100:GLU:HB2	1:G:130:MSE:HE3	2.03	0.40
1:G:166:LEU:HD11	1:G:262:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/318 (93%)	272 (92%)	20 (7%)	5 (2%)	7	27
1	B	297/318 (93%)	267 (90%)	21 (7%)	9 (3%)	3	15
1	C	297/318 (93%)	269 (91%)	25 (8%)	3 (1%)	13	40
1	D	297/318 (93%)	274 (92%)	19 (6%)	4 (1%)	10	33
1	E	297/318 (93%)	266 (90%)	27 (9%)	4 (1%)	10	33
1	F	297/318 (93%)	266 (90%)	28 (9%)	3 (1%)	13	40
1	G	297/318 (93%)	267 (90%)	22 (7%)	8 (3%)	4	17
1	H	297/318 (93%)	269 (91%)	27 (9%)	1 (0%)	37	66
All	All	2376/2544 (93%)	2150 (90%)	189 (8%)	37 (2%)	8	28

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	284	GLY
1	D	119	GLY
1	E	134	ASP
1	E	215	SER
1	F	25	GLN
1	G	40	VAL
1	G	93	ARG
1	A	92	GLY
1	B	93	ARG
1	B	119	GLY
1	B	282	SER
1	C	93	ARG
1	C	284	GLY
1	G	120	GLY
1	G	134	ASP
1	B	134	ASP
1	D	230	GLN
1	E	39	SER
1	F	134	ASP
1	G	92	GLY
1	G	228	LYS
1	A	134	ASP
1	A	236	GLU
1	B	215	SER
1	B	283	ALA
1	D	42	TYR
1	G	229	ALA
1	H	222	PHE
1	B	239	VAL
1	C	134	ASP
1	E	231	ASP
1	F	92	GLY
1	B	92	GLY
1	D	92	GLY
1	G	284	GLY
1	A	239	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	A	241/248 (97%)	232 (96%)	9 (4%)	29	64
1	B	241/248 (97%)	228 (95%)	13 (5%)	18	49
1	C	241/248 (97%)	222 (92%)	19 (8%)	10	30
1	D	241/248 (97%)	226 (94%)	15 (6%)	15	43
1	E	241/248 (97%)	228 (95%)	13 (5%)	18	49
1	F	241/248 (97%)	230 (95%)	11 (5%)	23	55
1	G	241/248 (97%)	229 (95%)	12 (5%)	20	52
1	H	241/248 (97%)	230 (95%)	11 (5%)	23	55
All	All	1928/1984 (97%)	1825 (95%)	103 (5%)	19	49

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	95	CYS
1	A	108	GLN
1	A	118	GLN
1	A	130	MSE
1	A	165	VAL
1	A	175	LEU
1	A	181	GLN
1	A	206	CYS
1	B	5	GLN
1	B	86	PHE
1	B	101	LEU
1	B	130	MSE
1	B	139	SER
1	B	175	LEU
1	B	176	GLN
1	B	197	VAL
1	B	199	THR
1	B	206	CYS
1	B	256	ARG
1	B	262	VAL
1	B	290	LEU
1	C	5	GLN
1	C	34	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	55	THR
1	C	85	SER
1	C	93	ARG
1	C	95	CYS
1	C	129	THR
1	C	130	MSE
1	C	143	CYS
1	C	147	PRO
1	C	149	MSE
1	C	154	ASP
1	C	157	ARG
1	C	175	LEU
1	C	204	GLU
1	C	206	CYS
1	C	207	LEU
1	C	262	VAL
1	C	290	LEU
1	D	85	SER
1	D	101	LEU
1	D	130	MSE
1	D	147	PRO
1	D	149	MSE
1	D	154	ASP
1	D	175	LEU
1	D	206	CYS
1	D	207	LEU
1	D	228	LYS
1	D	256	ARG
1	D	262	VAL
1	D	272	ILE
1	D	285	ASP
1	D	290	LEU
1	E	1	MSE
1	E	66	ASP
1	E	84	VAL
1	E	93	ARG
1	E	99	LYS
1	E	115	LYS
1	E	129	THR
1	E	130	MSE
1	E	143	CYS
1	E	165	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	166	LEU
1	E	175	LEU
1	E	206	CYS
1	F	5	GLN
1	F	73	ASN
1	F	84	VAL
1	F	121	SER
1	F	130	MSE
1	F	175	LEU
1	F	198	THR
1	F	199	THR
1	F	239	VAL
1	F	256	ARG
1	F	282	SER
1	G	26	THR
1	G	32	VAL
1	G	36	ASN
1	G	50	VAL
1	G	101	LEU
1	G	160	GLN
1	G	175	LEU
1	G	182	GLN
1	G	239	VAL
1	G	269	ARG
1	G	276	VAL
1	G	282	SER
1	H	5	GLN
1	H	50	VAL
1	H	79	GLU
1	H	94	THR
1	H	101	LEU
1	H	128	LEU
1	H	129	THR
1	H	157	ARG
1	H	175	LEU
1	H	222	PHE
1	H	297	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	72	GLN
1	A	112	GLN
1	A	118	GLN
1	A	158	ASN
1	A	181	GLN
1	A	296	ASN
1	B	52	ASN
1	B	72	GLN
1	B	74	HIS
1	B	75	GLN
1	B	140	HIS
1	B	141	HIS
1	B	230	GLN
1	B	296	ASN
1	C	112	GLN
1	C	158	ASN
1	C	181	GLN
1	D	27	HIS
1	D	72	GLN
1	D	176	GLN
1	D	181	GLN
1	D	182	GLN
1	D	296	ASN
1	E	23	HIS
1	E	25	GLN
1	E	158	ASN
1	E	182	GLN
1	E	296	ASN
1	F	5	GLN
1	F	27	HIS
1	F	72	GLN
1	F	73	ASN
1	F	158	ASN
1	F	181	GLN
1	G	36	ASN
1	G	108	GLN
1	G	112	GLN
1	G	140	HIS
1	G	158	ASN
1	G	182	GLN
1	G	230	GLN
1	G	238	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	296	ASN
1	H	5	GLN
1	H	23	HIS
1	H	27	HIS
1	H	72	GLN
1	H	108	GLN
1	H	230	GLN
1	H	297	HIS

### 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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	293/318 (92%)	-0.26	5 (1%) 69 63	25, 42, 64, 78	0
1	B	293/318 (92%)	-0.16	12 (4%) 42 35	26, 42, 66, 94	0
1	C	293/318 (92%)	-0.07	9 (3%) 51 46	26, 46, 73, 100	0
1	D	293/318 (92%)	0.12	18 (6%) 28 24	30, 48, 77, 100	0
1	E	293/318 (92%)	-0.04	8 (2%) 56 50	27, 48, 70, 85	0
1	F	293/318 (92%)	-0.25	8 (2%) 56 50	26, 42, 66, 91	0
1	G	293/318 (92%)	-0.15	12 (4%) 42 35	27, 41, 68, 88	0
1	H	293/318 (92%)	-0.10	13 (4%) 39 33	28, 41, 71, 95	0
All	All	2344/2544 (92%)	-0.11	85 (3%) 46 40	25, 44, 71, 100	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	229	ALA	5.5
1	G	42	TYR	4.5
1	C	148	TYR	4.5
1	H	119	GLY	4.4
1	C	299	SER	3.9
1	G	95	CYS	3.9
1	F	148	TYR	3.9
1	D	119	GLY	3.9
1	H	148	TYR	3.8
1	C	147	PRO	3.7
1	H	298	ALA	3.6
1	D	299	SER	3.5
1	D	121	SER	3.5
1	G	299	SER	3.5
1	D	148	TYR	3.5
1	B	148	TYR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	299	SER	3.3
1	D	227	ALA	3.3
1	G	227	ALA	3.3
1	H	155	ARG	3.3
1	H	227	ALA	3.2
1	D	120	GLY	3.1
1	H	120	GLY	3.1
1	A	92	GLY	3.1
1	G	38	LEU	3.1
1	D	68	VAL	3.0
1	B	93	ARG	3.0
1	B	43	GLY	3.0
1	C	2	GLU	3.0
1	D	42	TYR	2.9
1	D	226	VAL	2.9
1	H	297	HIS	2.9
1	F	298	ALA	2.9
1	C	121	SER	2.8
1	F	299	SER	2.8
1	B	118	GLN	2.8
1	B	42	TYR	2.8
1	G	94	THR	2.8
1	F	297	HIS	2.8
1	E	114	TYR	2.7
1	D	229	ALA	2.7
1	D	93	ARG	2.7
1	C	153	SER	2.7
1	E	94	THR	2.7
1	A	42	TYR	2.7
1	E	148	TYR	2.7
1	H	94	THR	2.7
1	D	150	PRO	2.6
1	A	299	SER	2.6
1	D	95	CYS	2.6
1	F	78	GLU	2.6
1	H	230	GLN	2.6
1	D	92	GLY	2.5
1	E	42	TYR	2.5
1	E	92	GLY	2.5
1	B	228	LYS	2.4
1	D	147	PRO	2.4
1	H	228	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	157	ARG	2.4
1	B	94	THR	2.4
1	D	94	THR	2.4
1	G	154	ASP	2.4
1	A	119	GLY	2.3
1	B	271	GLY	2.3
1	F	68	VAL	2.3
1	A	227	ALA	2.3
1	C	95	CYS	2.3
1	G	118	GLN	2.3
1	B	119	GLY	2.3
1	E	299	SER	2.3
1	E	41	ASN	2.3
1	F	158	ASN	2.3
1	B	95	CYS	2.3
1	H	157	ARG	2.2
1	D	79	GLU	2.2
1	D	3	THR	2.2
1	G	41	ASN	2.2
1	F	79	GLU	2.2
1	H	117	PRO	2.1
1	C	150	PRO	2.1
1	G	40	VAL	2.1
1	E	227	ALA	2.1
1	B	117	PRO	2.1
1	C	119	GLY	2.1
1	B	157	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	507	1/1	0.92	0.18	76,76,76,76	0
2	CL	G	505	1/1	0.92	0.18	63,63,63,63	0
2	CL	E	508	1/1	0.96	0.10	59,59,59,59	0
2	CL	A	509	1/1	0.96	0.08	61,61,61,61	0
2	CL	G	506	1/1	0.96	0.05	69,69,69,69	0
2	CL	H	504	1/1	0.96	0.15	63,63,63,63	0
2	CL	G	502	1/1	0.97	0.14	66,66,66,66	0
2	CL	C	501	1/1	0.98	0.16	52,52,52,52	0
2	CL	F	503	1/1	0.98	0.08	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.