



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:43 AM GMT

PDB ID : 3BUA  
Title : Crystal Structure of TRF2 TRFH domain and APOLLO peptide complex  
Authors : Chen, Y.; Yang, Y.; van Overbeek, M.; Donigian, J.R.; Baciú, P.; de Lange, T.; Lei, M.  
Deposited on : 2008-01-02  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

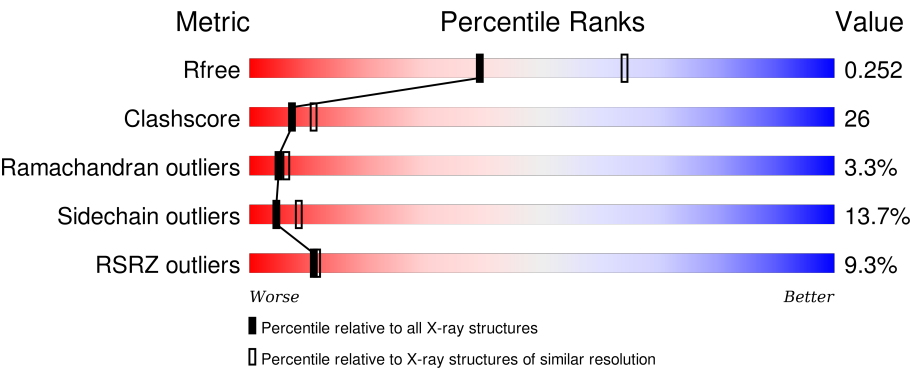
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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 <sub>free</sub>	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	204	<div><div>9%</div><div>53%</div><div>38%</div><div>6%</div><div>..</div></div>
1	B	204	<div><div>5%</div><div>60%</div><div>29%</div><div>8%</div><div>..</div></div>
1	C	204	<div><div>11%</div><div>60%</div><div>30%</div><div>8%</div><div>..</div></div>
1	D	204	<div><div>7%</div><div>50%</div><div>39%</div><div>9%</div><div>.</div></div>
2	E	36	<div><div>11%</div><div>14%</div><div>19%</div><div>6%</div><div>61%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	36	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%17%8%8%67%</div></div>
2	G	36	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>19%17%19%8%56%</div></div>
2	H	36	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%19%11%•67%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7148 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 Telomeric repeat-binding factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			
1	B	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			
1	C	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			
1	D	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			

- Molecule 2 is a protein called DNA cross-link repair 1B protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	0	0	0
			113	77	19	17			
2	F	12	Total	C	N	O	0	0	0
			94	64	16	14			
2	G	16	Total	C	N	O	0	0	0
			128	85	21	22			
2	H	12	Total	C	N	O	0	0	0
			91	62	14	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	495	SER	THR	SEE REMARK 999	UNP Q9H816
F	495	SER	THR	SEE REMARK 999	UNP Q9H816
G	495	SER	THR	SEE REMARK 999	UNP Q9H816
H	495	SER	THR	SEE REMARK 999	UNP Q9H816

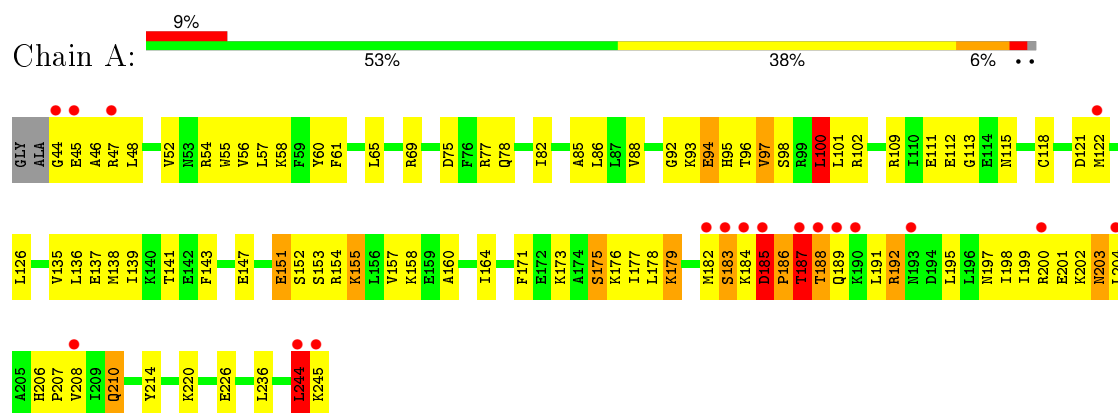
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	39	Total 39	O 39	0	0
3	C	24	Total 24	O 24	0	0
3	D	20	Total 20	O 20	0	0
3	E	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0

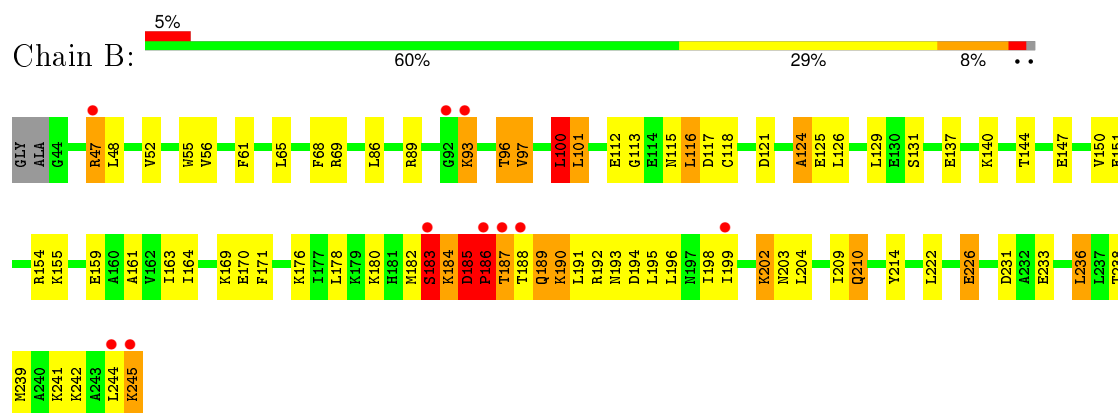
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

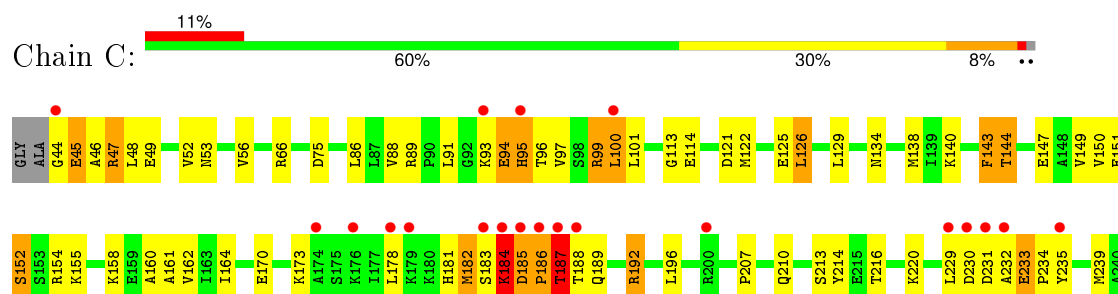
#### • Molecule 1: Telomeric repeat-binding factor 2

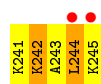


#### • Molecule 1: Telomeric repeat-binding factor 2

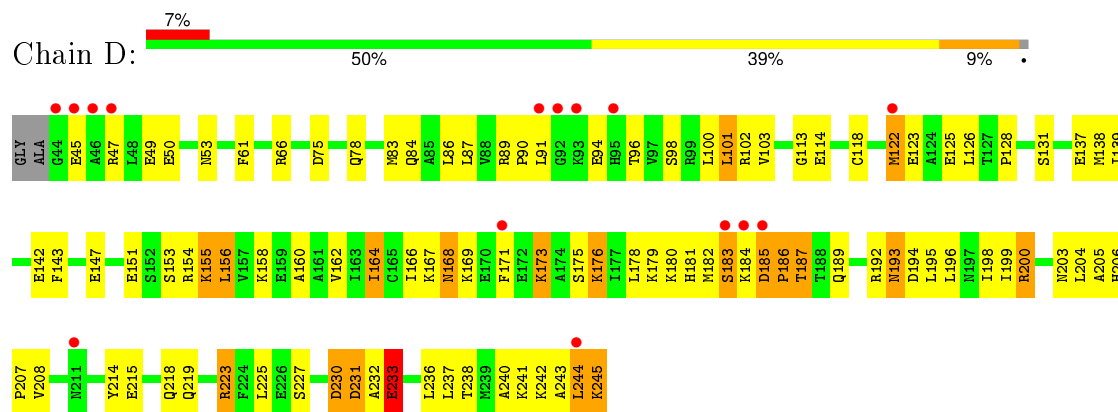


#### • Molecule 1: Telomeric repeat-binding factor 2

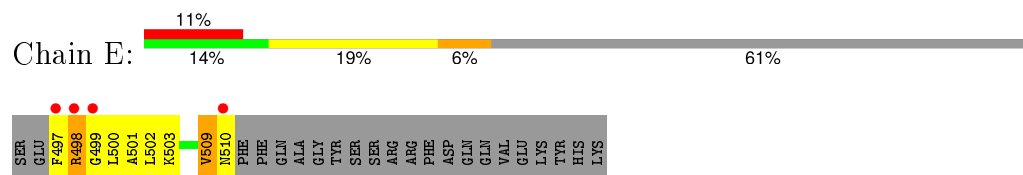




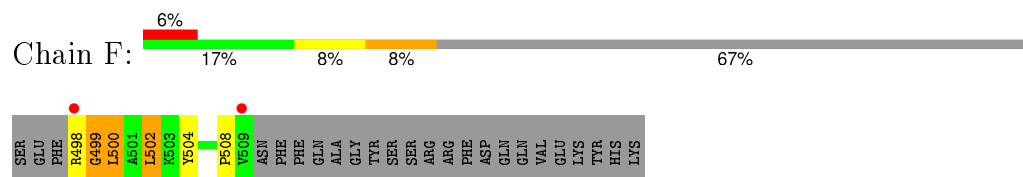
- Molecule 1: Telomeric repeat-binding factor 2



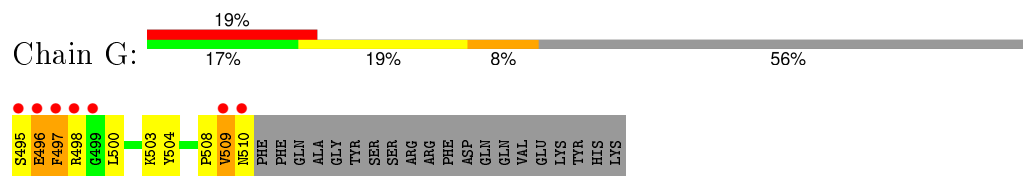
- Molecule 2: DNA cross-link repair 1B protein



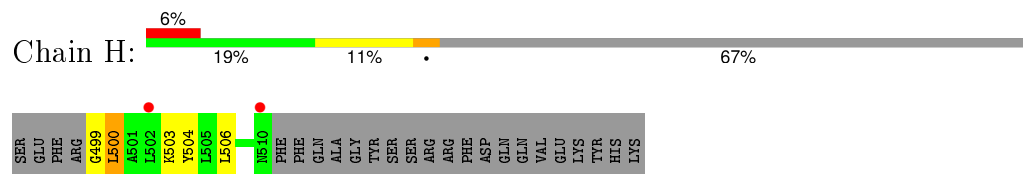
- Molecule 2: DNA cross-link repair 1B protein



- Molecule 2: DNA cross-link repair 1B protein



- Molecule 2: DNA cross-link repair 1B protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.95Å 109.95Å 130.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 42.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.50) 95.8 (42.09-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.254 0.228 , 0.252	Depositor DCC
$R_{free}$ test set	3069 reflections (10.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31885 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/1678	0.75	3/2249 (0.1%)
1	B	0.36	0/1678	0.73	4/2249 (0.2%)
1	C	0.33	0/1678	0.70	2/2249 (0.1%)
1	D	0.37	0/1678	0.74	2/2249 (0.1%)
2	E	0.51	0/115	0.87	0/155
2	F	0.36	0/95	0.79	1/128 (0.8%)
2	G	0.49	0/130	1.44	3/175 (1.7%)
2	H	0.39	0/92	0.83	0/125
All	All	0.36	0/7144	0.75	15/9579 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	LEU	CA-CB-CG	13.30	145.90	115.30
2	G	509	VAL	CB-CA-C	8.99	128.48	111.40
1	A	185	ASP	N-CA-C	7.58	131.48	111.00
1	B	185	ASP	N-CA-C	7.11	130.20	111.00
1	A	100	LEU	CA-CB-CG	6.46	130.17	115.30
1	D	233	GLU	N-CA-C	-6.39	93.75	111.00
2	G	496	GLU	N-CA-C	5.93	127.02	111.00
2	G	509	VAL	N-CA-C	-5.84	95.22	111.00
2	F	499	GLY	N-CA-C	-5.83	98.53	113.10
1	C	184	LYS	N-CA-C	-5.56	95.98	111.00
1	D	231	ASP	N-CA-C	-5.51	96.12	111.00
1	B	100	LEU	CA-CB-CG	5.50	127.95	115.30
1	B	124	ALA	N-CA-C	5.46	125.74	111.00
1	C	233	GLU	N-CA-C	-5.03	97.43	111.00
1	B	126	LEU	N-CA-C	-5.02	97.44	111.00

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	1653	0	1705	87	0
1	B	1653	0	1705	77	0
1	C	1653	0	1705	89	0
1	D	1653	0	1705	105	0
2	E	113	0	124	8	0
2	F	94	0	109	6	0
2	G	128	0	135	14	0
2	H	91	0	102	8	0
3	A	24	0	0	2	0
3	B	39	0	0	0	0
3	C	24	0	0	2	0
3	D	20	0	0	1	0
3	E	1	0	0	0	0
3	G	2	0	0	0	0
All	All	7148	0	7290	373	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 26.

All (373) 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:D:185:ASP:HB3	1:D:186:PRO:CD	1.74	1.17
2:G:508:PRO:HB2	2:G:510:ASN:ND2	1.64	1.11
1:D:185:ASP:HB3	1:D:186:PRO:HD3	1.17	1.10
1:A:185:ASP:O	1:A:189:GLN:HG3	1.52	1.10
1:C:93:LYS:HE3	1:C:95:HIS:ND1	1.69	1.05
2:G:508:PRO:HB2	2:G:510:ASN:HD21	1.23	1.01
1:D:91:LEU:HD12	2:H:500:LEU:HD12	1.42	1.01
1:B:183:SER:HB3	1:B:192:ARG:NH1	1.75	1.00
1:B:183:SER:HA	1:B:192:ARG:HD2	1.44	0.99
1:D:114:GLU:HG2	1:D:164:ILE:HD11	1.44	0.98
2:G:509:VAL:O	2:G:510:ASN:HB2	1.60	0.97
1:A:57:LEU:HD23	1:A:97:VAL:HG11	1.49	0.94
1:D:173:LYS:NZ	1:D:173:LYS:HB3	1.82	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:PRO:O	1:D:189:GLN:HG3	1.69	0.93
2:G:508:PRO:HB2	2:G:510:ASN:CG	1.88	0.93
1:D:179:LYS:HA	1:D:183:SER:HB3	1.48	0.93
1:D:185:ASP:CB	1:D:186:PRO:HD3	1.98	0.92
2:G:508:PRO:CB	2:G:510:ASN:OD1	2.18	0.92
1:A:183:SER:HA	1:A:192:ARG:NH1	1.86	0.91
1:C:230:ASP:O	1:C:232:ALA:N	2.02	0.91
1:C:66:ARG:HG2	1:C:66:ARG:HH11	1.37	0.89
1:A:185:ASP:O	1:A:189:GLN:CG	2.20	0.89
1:C:88:VAL:HA	2:G:498:ARG:O	1.74	0.88
1:D:195:LEU:O	1:D:199:ILE:HG13	1.73	0.88
1:A:179:LYS:O	1:A:183:SER:HB3	1.76	0.86
1:D:183:SER:HA	1:D:192:ARG:NH1	1.90	0.86
2:G:509:VAL:O	2:G:510:ASN:CB	2.24	0.85
2:G:508:PRO:HB3	2:G:510:ASN:OD1	1.76	0.85
1:D:243:ALA:C	1:D:245:LYS:H	1.79	0.85
1:C:184:LYS:O	1:C:186:PRO:N	2.09	0.85
1:C:186:PRO:O	1:C:189:GLN:HG3	1.77	0.85
1:B:93:LYS:HB2	1:B:96:THR:OG1	1.80	0.82
1:B:178:LEU:HD11	1:B:192:ARG:HG3	1.62	0.82
1:A:178:LEU:HD11	1:A:192:ARG:HG3	1.62	0.81
1:D:200:ARG:HH11	1:D:200:ARG:HG2	1.46	0.80
1:D:186:PRO:HG2	1:D:187:THR:H	1.45	0.80
1:B:183:SER:HB3	1:B:192:ARG:CZ	2.12	0.79
1:B:242:LYS:HA	1:B:245:LYS:HD2	1.64	0.79
1:C:243:ALA:C	1:C:244:LEU:HD23	2.02	0.79
1:D:194:ASP:O	1:D:198:ILE:HG13	1.82	0.79
1:B:97:VAL:CG1	1:B:101:LEU:HD22	2.12	0.79
1:D:186:PRO:CG	1:D:187:THR:H	1.94	0.78
2:G:508:PRO:HB2	2:G:510:ASN:OD1	1.82	0.78
1:C:184:LYS:HE2	1:C:184:LYS:HA	1.66	0.76
1:C:186:PRO:O	1:C:188:THR:N	2.19	0.75
1:B:182:MET:O	1:B:184:LYS:N	2.19	0.75
1:D:66:ARG:HG2	1:D:66:ARG:HH11	1.53	0.74
1:C:185:ASP:O	1:C:188:THR:HG22	1.87	0.73
1:C:244:LEU:N	1:C:244:LEU:HD23	2.01	0.73
1:C:178:LEU:HD12	1:C:182:MET:SD	2.28	0.73
1:C:93:LYS:HE3	1:C:95:HIS:CE1	2.23	0.73
1:A:54:ARG:NH1	1:A:93:LYS:NZ	2.36	0.73
1:A:55:TRP:HB3	1:A:236:LEU:HD13	1.69	0.73
1:A:182:MET:O	1:A:192:ARG:HD2	1.89	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:O	1:A:58:LYS:HG3	1.89	0.72
1:A:122:MET:HA	1:A:122:MET:HE3	1.71	0.72
1:B:195:LEU:O	1:B:199:ILE:HG13	1.89	0.72
1:D:178:LEU:HD13	1:D:182:MET:HE1	1.71	0.72
1:B:185:ASP:O	1:B:186:PRO:O	2.08	0.72
2:F:499:GLY:O	2:F:502:LEU:N	2.18	0.71
1:D:173:LYS:HB3	1:D:173:LYS:HZ1	1.53	0.71
1:A:185:ASP:O	1:A:186:PRO:O	2.08	0.70
1:B:116:LEU:HD12	1:B:170:GLU:HG3	1.73	0.70
1:D:243:ALA:C	1:D:245:LYS:N	2.44	0.70
1:A:187:THR:C	1:A:189:GLN:H	1.95	0.70
1:C:100:LEU:HD23	1:C:101:LEU:N	2.06	0.70
1:B:183:SER:CA	1:B:192:ARG:HD2	2.20	0.70
1:D:200:ARG:O	1:D:200:ARG:HD3	1.92	0.70
1:D:233:GLU:OE2	1:D:241:LYS:NZ	2.24	0.69
1:A:57:LEU:HD23	1:A:97:VAL:CG1	2.22	0.69
1:C:93:LYS:O	1:C:96:THR:HG22	1.92	0.69
1:D:169:LYS:HA	1:D:171:PHE:CE1	2.26	0.69
1:C:185:ASP:OD1	1:C:188:THR:HG21	1.92	0.69
1:C:66:ARG:HG2	1:C:66:ARG:NH1	2.02	0.68
1:A:183:SER:HA	1:A:192:ARG:HH11	1.57	0.68
2:F:498:ARG:HG3	2:F:499:GLY:N	2.06	0.68
1:D:182:MET:O	1:D:192:ARG:HD2	1.94	0.68
1:D:185:ASP:CB	1:D:186:PRO:CD	2.59	0.68
1:C:44:GLY:C	1:C:46:ALA:H	1.96	0.68
1:D:206:HIS:CE1	1:D:208:VAL:HG23	2.28	0.68
1:C:147:GLU:OE1	1:C:154:ARG:NH2	2.27	0.68
1:A:244:LEU:O	1:A:245:LYS:C	2.32	0.68
1:C:100:LEU:HD23	1:C:100:LEU:C	2.14	0.67
1:C:184:LYS:O	1:C:185:ASP:C	2.32	0.67
1:D:101:LEU:HB3	2:H:504:TYR:CD2	2.29	0.67
1:B:199:ILE:O	1:B:202:LYS:HD3	1.95	0.66
1:D:182:MET:O	1:D:184:LYS:N	2.26	0.66
1:B:242:LYS:CA	1:B:245:LYS:HD2	2.26	0.66
1:A:154:ARG:HG2	1:A:158:LYS:HE3	1.75	0.66
1:D:151:GLU:O	1:D:155:LYS:HB2	1.96	0.66
1:D:78:GLN:NE2	2:G:497:PHE:O	2.28	0.65
1:A:185:ASP:O	1:A:189:GLN:CD	2.35	0.65
1:B:159:GLU:O	1:B:163:ILE:HG13	1.96	0.65
1:A:122:MET:O	2:H:503:LYS:HG3	1.96	0.65
1:B:97:VAL:HG12	1:B:101:LEU:HD22	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:499:GLY:O	2:E:502:LEU:N	2.28	0.65
1:C:94:GLU:OE2	2:G:503:LYS:NZ	2.23	0.64
1:D:231:ASP:OD2	1:D:232:ALA:N	2.30	0.64
1:D:94:GLU:CG	1:D:94:GLU:O	2.45	0.64
1:B:185:ASP:O	1:B:189:GLN:NE2	2.28	0.64
1:B:187:THR:O	1:B:187:THR:HG23	1.96	0.64
1:A:186:PRO:O	1:A:189:GLN:N	2.30	0.63
1:D:182:MET:C	1:D:184:LYS:H	2.02	0.63
1:B:198:ILE:HG23	1:B:203:ASN:O	1.97	0.63
1:D:114:GLU:HA	1:D:164:ILE:HD12	1.78	0.63
1:A:147:GLU:O	1:A:151:GLU:HG2	1.99	0.63
1:A:151:GLU:O	1:A:155:LYS:HG2	1.99	0.63
1:D:183:SER:HA	1:D:192:ARG:CZ	2.28	0.62
1:C:187:THR:HA	1:C:189:GLN:CD	2.19	0.62
2:E:509:VAL:HG12	2:E:510:ASN:N	2.14	0.62
1:C:99:ARG:HG3	1:C:143:PHE:CZ	2.34	0.62
1:C:44:GLY:C	1:C:46:ALA:N	2.53	0.62
1:B:100:LEU:HD22	1:B:101:LEU:N	2.14	0.62
1:A:178:LEU:HD11	1:A:192:ARG:CG	2.29	0.62
1:A:85:ALA:O	1:A:88:VAL:HG22	2.00	0.62
1:C:182:MET:O	1:C:192:ARG:HD2	1.99	0.61
1:D:214:TYR:O	1:D:218:GLN:HG3	2.00	0.61
1:D:200:ARG:HG2	1:D:200:ARG:NH1	2.10	0.61
1:A:113:GLY:HA3	1:A:214:TYR:OH	2.01	0.61
1:C:99:ARG:HH11	1:C:99:ARG:HG2	1.66	0.61
1:B:69:ARG:NH2	1:B:226:GLU:OE2	2.30	0.61
1:B:101:LEU:HB3	2:F:504:TYR:CD2	2.35	0.61
1:B:222:LEU:O	1:B:226:GLU:HB2	2.01	0.60
1:B:52:VAL:O	1:B:56:VAL:HG23	2.01	0.60
1:C:187:THR:C	1:C:189:GLN:H	2.05	0.60
1:D:179:LYS:O	1:D:183:SER:OG	2.19	0.60
1:D:183:SER:HA	1:D:192:ARG:HH11	1.67	0.60
1:D:114:GLU:HA	1:D:164:ILE:CD1	2.31	0.60
1:A:154:ARG:O	1:A:158:LYS:HG3	2.02	0.60
1:D:66:ARG:HG2	1:D:66:ARG:NH1	2.17	0.59
1:D:231:ASP:O	1:D:232:ALA:HB2	2.03	0.59
1:D:160:ALA:O	1:D:164:ILE:HB	2.02	0.59
1:A:45:GLU:HA	1:A:48:LEU:HD12	1.84	0.59
1:A:75:ASP:OD1	1:B:89:ARG:NH2	2.36	0.59
1:C:232:ALA:O	1:C:234:PRO:HD3	2.02	0.59
1:C:89:ARG:NH2	1:D:75:ASP:OD1	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLN:NE2	2:H:506:LEU:H	2.00	0.59
1:D:193:ASN:HD22	1:D:193:ASN:N	2.00	0.58
1:B:178:LEU:HD21	1:B:196:LEU:HG	1.84	0.58
1:D:183:SER:HA	1:D:192:ARG:HD2	1.84	0.58
1:D:185:ASP:HB3	1:D:186:PRO:HD2	1.78	0.58
1:A:147:GLU:OE1	1:A:154:ARG:NH2	2.37	0.58
1:C:186:PRO:C	1:C:188:THR:H	2.06	0.58
1:C:187:THR:HA	1:C:189:GLN:NE2	2.19	0.58
1:A:245:LYS:O	1:A:245:LYS:CG	2.51	0.58
1:A:100:LEU:HD23	1:A:101:LEU:N	2.19	0.57
1:A:137:GLU:OE2	1:A:154:ARG:NH1	2.37	0.57
1:D:186:PRO:CG	1:D:187:THR:N	2.67	0.57
1:A:186:PRO:O	1:A:187:THR:C	2.42	0.57
1:A:188:THR:O	1:A:192:ARG:HB2	2.05	0.57
1:D:178:LEU:HD12	1:D:182:MET:HB2	1.85	0.57
1:D:178:LEU:HD21	1:D:196:LEU:HG	1.87	0.57
1:D:183:SER:CA	1:D:192:ARG:NH1	2.66	0.57
1:C:170:GLU:HB3	1:C:173:LYS:HB2	1.87	0.57
1:D:84:GLN:HE22	2:H:506:LEU:H	1.53	0.56
1:C:207:PRO:HA	1:C:210:GLN:HB2	1.86	0.56
1:A:245:LYS:O	1:A:245:LYS:HG2	2.05	0.56
1:A:97:VAL:O	1:A:100:LEU:HD22	2.06	0.56
1:A:69:ARG:NH2	1:A:226:GLU:OE2	2.29	0.56
1:C:56:VAL:HG12	1:C:86:LEU:HD11	1.86	0.56
2:H:503:LYS:HD3	2:H:504:TYR:CE1	2.40	0.56
1:C:188:THR:HG23	1:C:188:THR:O	2.05	0.56
1:D:113:GLY:HA2	1:D:128:PRO:HB2	1.88	0.56
2:E:498:ARG:C	2:E:500:LEU:N	2.59	0.56
1:A:187:THR:O	1:A:189:GLN:N	2.39	0.55
1:B:190:LYS:HE3	1:B:194:ASP:OD2	2.06	0.55
1:C:93:LYS:CE	1:C:95:HIS:ND1	2.59	0.55
1:C:164:ILE:HD11	1:C:214:TYR:HD1	1.71	0.55
1:D:164:ILE:O	1:D:168:ASN:HB2	2.06	0.55
1:B:242:LYS:HA	1:B:245:LYS:CD	2.37	0.55
1:D:168:ASN:O	1:D:169:LYS:HB2	2.06	0.55
1:C:48:LEU:O	1:C:52:VAL:HG23	2.07	0.55
1:A:187:THR:C	1:A:189:GLN:N	2.59	0.55
1:D:182:MET:C	1:D:184:LYS:N	2.60	0.55
1:C:185:ASP:O	1:C:188:THR:CG2	2.54	0.55
1:D:138:MET:O	1:D:142:GLU:HG3	2.07	0.55
1:C:93:LYS:CE	1:C:95:HIS:CE1	2.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HG23	1:B:189:GLN:N	2.21	0.55
1:A:185:ASP:O	1:A:189:GLN:NE2	2.40	0.55
1:C:95:HIS:CG	1:C:96:THR:N	2.75	0.54
1:A:186:PRO:O	1:A:188:THR:N	2.40	0.54
1:A:173:LYS:O	1:A:177:ILE:HG13	2.06	0.54
1:B:183:SER:HA	1:B:192:ARG:CD	2.26	0.54
1:D:178:LEU:HD13	1:D:182:MET:CE	2.36	0.54
1:C:99:ARG:HG2	1:C:99:ARG:NH1	2.21	0.54
1:C:44:GLY:O	1:C:46:ALA:N	2.41	0.54
1:B:242:LYS:O	1:B:245:LYS:HD2	2.07	0.54
1:C:160:ALA:O	1:C:164:ILE:HG12	2.09	0.53
1:D:153:SER:O	1:D:156:LEU:HB2	2.08	0.53
1:C:178:LEU:HD21	1:C:196:LEU:HG	1.91	0.53
1:C:152:SER:HB2	3:C:559:HOH:O	2.08	0.53
1:C:244:LEU:CD2	1:C:244:LEU:N	2.71	0.53
1:A:54:ARG:NH1	1:A:93:LYS:HZ2	2.06	0.53
1:A:188:THR:O	1:A:188:THR:HG22	2.10	0.52
1:C:241:LYS:O	1:C:245:LYS:HB3	2.09	0.52
1:C:164:ILE:HD11	1:C:214:TYR:CD1	2.44	0.52
1:C:75:ASP:OD1	1:D:89:ARG:NH2	2.42	0.52
1:A:48:LEU:O	1:A:52:VAL:HG23	2.10	0.52
1:B:202:LYS:HD3	1:B:202:LYS:N	2.24	0.52
1:A:54:ARG:CZ	1:A:93:LYS:HE3	2.39	0.52
1:A:54:ARG:HH12	1:A:93:LYS:HZ1	1.58	0.52
1:D:237:LEU:O	1:D:237:LEU:HD12	2.10	0.52
1:A:60:TYR:OH	1:B:86:LEU:HD21	2.09	0.52
1:D:50:GLU:HG3	1:D:90:PRO:HB2	1.92	0.52
2:F:498:ARG:CG	2:F:499:GLY:N	2.73	0.52
1:D:94:GLU:C	3:D:570:HOH:O	2.48	0.52
1:A:115:ASN:O	1:A:118:CYS:HB3	2.10	0.51
1:C:235:TYR:O	1:C:239:MET:HG2	2.11	0.51
1:D:94:GLU:HG2	1:D:94:GLU:O	2.11	0.51
1:C:95:HIS:CD2	1:C:95:HIS:C	2.82	0.51
1:B:239:MET:HE2	1:B:239:MET:HA	1.91	0.51
1:A:139:ILE:O	1:A:143:PHE:HB2	2.10	0.51
1:A:192:ARG:NH2	3:A:603:HOH:O	2.44	0.51
1:D:179:LYS:HA	1:D:183:SER:CB	2.32	0.51
1:C:241:LYS:C	1:C:243:ALA:H	2.14	0.51
1:B:118:CYS:SG	2:F:508:PRO:HB3	2.50	0.51
1:C:184:LYS:C	1:C:186:PRO:N	2.65	0.51
2:E:499:GLY:C	2:E:501:ALA:N	2.63	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HA	1:B:210:GLN:HE21	1.75	0.50
1:D:240:ALA:O	1:D:244:LEU:HB2	2.11	0.50
1:B:113:GLY:HA3	1:B:214:TYR:OH	2.11	0.50
1:D:166:ILE:C	1:D:168:ASN:H	2.13	0.50
2:H:499:GLY:O	2:H:503:LYS:N	2.28	0.50
1:C:143:PHE:N	1:C:143:PHE:CD1	2.80	0.50
1:C:186:PRO:C	1:C:189:GLN:HG3	2.30	0.50
1:C:143:PHE:N	1:C:143:PHE:HD1	2.10	0.50
1:B:159:GLU:HA	1:B:182:MET:HE1	1.93	0.49
1:B:171:PHE:CD2	1:B:202:LYS:HD2	2.46	0.49
2:E:499:GLY:O	2:E:503:LYS:N	2.30	0.49
1:B:210:GLN:HE21	1:B:210:GLN:CA	2.24	0.49
1:C:147:GLU:CD	1:C:154:ARG:HH22	2.16	0.49
1:D:178:LEU:HD11	1:D:192:ARG:HG2	1.95	0.49
1:D:200:ARG:CG	1:D:200:ARG:HH11	2.22	0.49
1:C:46:ALA:O	1:C:48:LEU:N	2.46	0.49
1:A:244:LEU:O	1:A:245:LYS:O	2.31	0.49
1:C:53:ASN:HB3	1:C:91:LEU:HD23	1.94	0.49
1:B:147:GLU:OE2	1:B:154:ARG:NH2	2.46	0.49
1:A:178:LEU:HD12	1:A:178:LEU:O	2.12	0.49
1:C:113:GLY:HA3	1:C:214:TYR:OH	2.13	0.48
1:D:137:GLU:OE2	1:D:154:ARG:NH1	2.46	0.48
1:A:77:ARG:HD3	1:A:111:GLU:OE1	2.12	0.48
1:D:178:LEU:O	1:D:183:SER:N	2.47	0.48
1:B:61:PHE:CE2	1:B:100:LEU:HB2	2.48	0.48
1:A:102:ARG:NH2	1:D:123:GLU:O	2.47	0.48
1:B:188:THR:CG2	1:B:189:GLN:N	2.76	0.48
1:B:140:LYS:HB2	1:B:150:VAL:HG21	1.94	0.48
1:B:198:ILE:HD13	1:B:209:ILE:HG12	1.96	0.48
2:G:508:PRO:CB	2:G:510:ASN:CG	2.65	0.48
1:C:134:ASN:O	1:C:138:MET:HG3	2.14	0.47
1:C:186:PRO:O	1:C:189:GLN:N	2.48	0.47
1:D:169:LYS:HE3	1:D:204:LEU:HD11	1.96	0.47
1:D:166:ILE:C	1:D:168:ASN:N	2.67	0.47
1:B:242:LYS:O	1:B:245:LYS:CD	2.63	0.47
1:B:116:LEU:HD21	1:B:164:ILE:HG22	1.96	0.47
1:D:98:SER:O	1:D:102:ARG:HG2	2.15	0.47
1:C:144:THR:OG1	1:C:144:THR:O	2.24	0.47
1:D:103:VAL:HG13	1:D:225:LEU:HB3	1.95	0.47
1:C:232:ALA:O	1:C:234:PRO:CD	2.63	0.47
1:A:44:GLY:C	1:A:46:ALA:N	2.68	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:PRO:HG2	1:D:187:THR:HG22	1.97	0.47
2:E:498:ARG:C	2:E:500:LEU:H	2.17	0.47
1:C:185:ASP:N	1:C:186:PRO:HD3	2.31	0.46
1:C:140:LYS:NZ	1:C:147:GLU:OE2	2.48	0.46
1:A:186:PRO:C	1:A:188:THR:N	2.66	0.46
1:D:231:ASP:CG	1:D:232:ALA:N	2.69	0.46
1:B:185:ASP:O	1:B:186:PRO:C	2.46	0.46
1:A:135:VAL:HA	1:A:138:MET:CE	2.45	0.46
1:A:186:PRO:HA	1:A:189:GLN:NE2	2.30	0.46
1:A:100:LEU:C	1:A:100:LEU:HD23	2.36	0.46
1:A:183:SER:HA	1:A:192:ARG:HH12	1.77	0.46
1:C:184:LYS:HB2	1:C:185:ASP:H	1.55	0.46
1:A:93:LYS:HB3	1:A:96:THR:OG1	2.14	0.46
1:C:46:ALA:O	1:C:49:GLU:N	2.46	0.46
1:D:219:GLN:O	1:D:223:ARG:HG2	2.15	0.46
1:B:137:GLU:OE2	1:B:154:ARG:NH1	2.48	0.46
1:A:61:PHE:CE2	1:A:65:LEU:HD11	2.51	0.46
1:D:147:GLU:OE1	1:D:154:ARG:NH2	2.49	0.46
1:A:153:SER:O	1:A:157:VAL:HG23	2.16	0.46
1:D:158:LYS:HG2	1:D:181:HIS:HB3	1.98	0.45
1:B:68:PHE:HD2	1:B:222:LEU:HD22	1.82	0.45
1:B:61:PHE:CZ	1:B:65:LEU:HD11	2.51	0.45
1:A:171:PHE:HB3	1:A:199:ILE:HG23	1.99	0.45
1:D:203:ASN:OD1	1:D:205:ALA:HB3	2.16	0.45
1:A:199:ILE:O	1:A:202:LYS:HD3	2.16	0.45
1:B:183:SER:C	1:B:184:LYS:O	2.52	0.45
1:D:203:ASN:C	1:D:205:ALA:H	2.19	0.45
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.87	0.44
1:C:95:HIS:CD2	1:C:96:THR:N	2.86	0.44
1:A:54:ARG:NH1	1:A:93:LYS:CE	2.81	0.44
1:D:83:MET:O	1:D:87:LEU:HG	2.18	0.44
1:B:188:THR:O	1:B:191:LEU:N	2.49	0.44
1:C:140:LYS:HB2	1:C:150:VAL:HG21	1.98	0.44
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.83	0.44
1:A:210:GLN:HE21	1:A:210:GLN:CA	2.29	0.44
1:A:191:LEU:O	1:A:195:LEU:HG	2.16	0.44
1:D:183:SER:HA	1:D:192:ARG:CD	2.48	0.44
1:B:100:LEU:CD2	1:B:101:LEU:HD13	2.47	0.44
1:D:206:HIS:HA	1:D:207:PRO:HD3	1.95	0.44
1:B:129:LEU:CD1	1:B:161:ALA:HA	2.48	0.44
1:D:162:VAL:HG21	1:D:182:MET:HE2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLU:HG2	2:E:503:LYS:O	2.17	0.44
1:B:147:GLU:OE1	1:B:154:ARG:NH2	2.51	0.44
1:D:122:MET:HG2	2:E:502:LEU:HB3	1.98	0.44
1:D:61:PHE:CD2	1:D:100:LEU:HG	2.51	0.44
1:B:192:ARG:O	1:B:196:LEU:HD12	2.17	0.43
1:D:166:ILE:HD11	1:D:199:ILE:HG12	1.99	0.43
1:B:169:LYS:HG3	1:B:171:PHE:CE1	2.53	0.43
1:D:204:LEU:HD23	1:D:204:LEU:N	2.33	0.43
1:C:100:LEU:CD2	1:C:100:LEU:C	2.83	0.43
2:G:496:GLU:HB3	2:G:497:PHE:H	1.49	0.43
1:C:114:GLU:HB2	3:C:524:HOH:O	2.18	0.43
1:B:101:LEU:HA	1:B:101:LEU:HD12	1.83	0.43
1:B:187:THR:CG2	1:B:187:THR:O	2.65	0.43
1:B:245:LYS:HG3	1:B:245:LYS:H	1.71	0.43
1:B:100:LEU:C	1:B:100:LEU:CD2	2.87	0.43
2:F:499:GLY:O	2:F:500:LEU:C	2.57	0.43
1:D:203:ASN:C	1:D:205:ALA:N	2.72	0.43
2:G:500:LEU:HB3	2:G:504:TYR:HD1	1.83	0.43
1:A:179:LYS:NZ	3:A:603:HOH:O	2.51	0.43
1:C:229:LEU:HB3	1:C:230:ASP:H	1.66	0.43
1:A:58:LYS:NZ	1:A:96:THR:HG22	2.34	0.43
1:D:147:GLU:CD	1:D:154:ARG:HH22	2.21	0.43
1:C:241:LYS:C	1:C:243:ALA:N	2.71	0.42
1:B:112:GLU:OE1	1:B:115:ASN:ND2	2.52	0.42
1:C:93:LYS:O	1:C:94:GLU:C	2.58	0.42
1:D:49:GLU:HG2	1:D:53:ASN:HD21	1.84	0.42
1:B:56:VAL:HG12	1:B:86:LEU:HD11	2.02	0.42
1:C:121:ASP:OD1	1:C:126:LEU:HB2	2.19	0.42
1:A:175:SER:O	1:A:179:LYS:HB2	2.18	0.42
1:B:124:ALA:HB1	1:B:125:GLU:H	1.49	0.42
1:A:82:ILE:HD11	1:B:89:ARG:HG3	2.01	0.42
1:A:141:THR:OG1	1:D:176:LYS:NZ	2.53	0.42
1:C:151:GLU:O	1:C:155:LYS:HB2	2.18	0.42
1:B:186:PRO:O	1:B:189:GLN:NE2	2.53	0.42
1:C:97:VAL:O	1:C:100:LEU:HD22	2.20	0.42
1:B:68:PHE:CD2	1:B:222:LEU:HD22	2.54	0.42
1:B:210:GLN:HG3	1:C:216:THR:HG21	2.02	0.42
1:A:197:ASN:O	1:A:201:GLU:HG3	2.20	0.42
1:A:206:HIS:CE1	1:A:208:VAL:HG23	2.55	0.42
1:B:47:ARG:HA	1:B:47:ARG:HD3	1.82	0.42
1:D:233:GLU:OE1	1:D:238:THR:OG1	2.29	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:HG21	1:D:182:MET:CE	2.50	0.42
1:A:52:VAL:O	1:A:56:VAL:HG23	2.19	0.42
1:D:49:GLU:OE1	1:D:89:ARG:NH1	2.48	0.42
1:A:112:GLU:OE1	1:A:115:ASN:ND2	2.42	0.42
1:D:215:GLU:HA	1:D:218:GLN:HE21	1.84	0.42
1:A:206:HIS:ND1	1:A:207:PRO:HD2	2.34	0.42
1:B:100:LEU:CD2	1:B:101:LEU:N	2.80	0.41
1:C:241:LYS:O	1:C:243:ALA:N	2.53	0.41
1:B:55:TRP:HB3	1:B:236:LEU:HD13	2.02	0.41
1:C:241:LYS:O	1:C:245:LYS:CB	2.68	0.41
1:B:180:LYS:HG3	1:B:180:LYS:O	2.20	0.41
1:D:91:LEU:HD12	2:H:500:LEU:CD1	2.31	0.41
1:D:94:GLU:HG3	1:D:94:GLU:O	2.19	0.41
1:C:158:LYS:HE2	1:C:181:HIS:HB3	2.03	0.41
1:D:139:ILE:O	1:D:143:PHE:HB2	2.20	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.94	0.41
1:A:94:GLU:C	1:A:96:THR:H	2.25	0.41
1:A:54:ARG:NH1	1:A:93:LYS:HZ1	2.12	0.41
1:B:233:GLU:OE2	1:B:241:LYS:NZ	2.44	0.41
1:A:198:ILE:HG23	1:A:203:ASN:O	2.20	0.41
1:D:244:LEU:HA	1:D:244:LEU:HD22	1.96	0.41
1:A:78:GLN:O	1:A:82:ILE:HG13	2.21	0.40
1:C:121:ASP:CG	1:C:126:LEU:HB2	2.42	0.40
1:C:46:ALA:C	1:C:48:LEU:N	2.74	0.40
1:B:48:LEU:O	1:B:52:VAL:HG23	2.21	0.40
1:C:129:LEU:HD13	1:C:161:ALA:HA	2.01	0.40
1:C:186:PRO:C	1:C:188:THR:N	2.69	0.40
1:B:194:ASP:O	1:B:198:ILE:HG13	2.21	0.40
1:C:158:LYS:O	1:C:162:VAL:HG23	2.20	0.40
1:B:238:THR:HG22	1:B:239:MET:CE	2.51	0.40
1:D:180:LYS:HG2	1:D:181:HIS:CD2	2.57	0.40
1:A:160:ALA:O	1:A:164:ILE:HG12	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/204 (98%)	187 (94%)	6 (3%)	7 (4%)	4	6
1	B	200/204 (98%)	183 (92%)	12 (6%)	5 (2%)	7	10
1	C	200/204 (98%)	178 (89%)	12 (6%)	10 (5%)	3	3
1	D	200/204 (98%)	185 (92%)	10 (5%)	5 (2%)	7	10
2	E	12/36 (33%)	11 (92%)	1 (8%)	0	100	100
2	F	10/36 (28%)	8 (80%)	2 (20%)	0	100	100
2	G	14/36 (39%)	11 (79%)	2 (14%)	1 (7%)	1	1
2	H	10/36 (28%)	9 (90%)	1 (10%)	0	100	100
All	All	846/960 (88%)	772 (91%)	46 (5%)	28 (3%)	5	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	186	PRO
1	B	183	SER
1	B	186	PRO
1	B	189	GLN
1	C	186	PRO
1	C	187	THR
1	C	231	ASP
1	D	185	ASP
1	D	186	PRO
1	A	188	THR
1	C	47	ARG
1	D	183	SER
1	D	187	THR
1	D	230	ASP
1	A	92	GLY
1	A	184	LYS
1	A	187	THR
1	C	45	GLU
2	G	497	PHE
1	A	95	HIS
1	B	184	LYS
1	C	185	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	242	LYS
1	C	94	GLU
1	C	184	LYS
1	C	233	GLU
1	B	185	ASP

### 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	182/182 (100%)	158 (87%)	24 (13%)	5	9
1	B	182/182 (100%)	155 (85%)	27 (15%)	4	7
1	C	182/182 (100%)	162 (89%)	20 (11%)	8	14
1	D	182/182 (100%)	154 (85%)	28 (15%)	3	6
2	E	12/32 (38%)	9 (75%)	3 (25%)	1	1
2	F	10/32 (31%)	8 (80%)	2 (20%)	1	3
2	G	14/32 (44%)	13 (93%)	1 (7%)	18	34
2	H	10/32 (31%)	9 (90%)	1 (10%)	9	18
All	All	774/856 (90%)	668 (86%)	106 (14%)	4	8

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	86	LEU
1	A	94	GLU
1	A	97	VAL
1	A	98	SER
1	A	100	LEU
1	A	121	ASP
1	A	126	LEU
1	A	151	GLU
1	A	152	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	155	LYS
1	A	175	SER
1	A	176	LYS
1	A	179	LYS
1	A	183	SER
1	A	185	ASP
1	A	187	THR
1	A	192	ARG
1	A	200	ARG
1	A	203	ASN
1	A	204	LEU
1	A	210	GLN
1	A	220	LYS
1	A	244	LEU
1	B	47	ARG
1	B	93	LYS
1	B	96	THR
1	B	97	VAL
1	B	100	LEU
1	B	101	LEU
1	B	116	LEU
1	B	117	ASP
1	B	121	ASP
1	B	131	SER
1	B	144	THR
1	B	151	GLU
1	B	155	LYS
1	B	176	LYS
1	B	183	SER
1	B	186	PRO
1	B	187	THR
1	B	190	LYS
1	B	193	ASN
1	B	202	LYS
1	B	204	LEU
1	B	210	GLN
1	B	226	GLU
1	B	231	ASP
1	B	236	LEU
1	B	244	LEU
1	B	245	LYS
1	C	45	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	47	ARG
1	C	95	HIS
1	C	99	ARG
1	C	100	LEU
1	C	122	MET
1	C	125	GLU
1	C	126	LEU
1	C	143	PHE
1	C	144	THR
1	C	149	VAL
1	C	152	SER
1	C	182	MET
1	C	183	SER
1	C	187	THR
1	C	192	ARG
1	C	213	SER
1	C	220	LYS
1	C	242	LYS
1	C	244	LEU
1	D	45	GLU
1	D	47	ARG
1	D	86	LEU
1	D	96	THR
1	D	101	LEU
1	D	118	CYS
1	D	122	MET
1	D	125	GLU
1	D	126	LEU
1	D	131	SER
1	D	155	LYS
1	D	156	LEU
1	D	164	ILE
1	D	167	LYS
1	D	168	ASN
1	D	173	LYS
1	D	175	SER
1	D	176	LYS
1	D	193	ASN
1	D	200	ARG
1	D	223	ARG
1	D	227	SER
1	D	230	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	233	GLU
1	D	236	LEU
1	D	242	LYS
1	D	244	LEU
1	D	245	LYS
2	E	497	PHE
2	E	498	ARG
2	E	509	VAL
2	F	500	LEU
2	F	502	LEU
2	G	495	SER
2	H	500	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	197	ASN
1	A	203	ASN
1	A	210	GLN
1	A	218	GLN
1	B	210	GLN
1	B	211	ASN
1	B	218	GLN
1	B	228	HIS
1	D	84	GLN
1	D	193	ASN
1	D	218	GLN
1	D	219	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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, 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	202/204 (99%)	0.40	18 (8%) 12 13	29, 44, 72, 94	0
1	B	202/204 (99%)	0.32	10 (4%) 32 37	28, 43, 66, 86	0
1	C	202/204 (99%)	0.59	22 (10%) 7 7	29, 47, 78, 91	0
1	D	202/204 (99%)	0.46	15 (7%) 17 19	33, 56, 77, 88	0
2	E	14/36 (38%)	1.50	4 (28%) 1 0	35, 42, 78, 84	0
2	F	12/36 (33%)	0.71	2 (16%) 2 2	33, 42, 69, 83	0
2	G	16/36 (44%)	2.11	7 (43%) 0 0	33, 49, 82, 85	0
2	H	12/36 (33%)	0.73	2 (16%) 2 2	38, 45, 59, 69	0
All	All	862/960 (89%)	0.50	80 (9%) 11 11	28, 48, 77, 94	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	510	ASN	8.2
1	A	183	SER	6.5
2	E	497	PHE	6.5
2	G	495	SER	5.8
1	C	184	LYS	5.7
1	A	188	THR	5.6
1	B	245	LYS	5.5
1	A	185	ASP	5.3
1	C	185	ASP	5.2
1	C	188	THR	5.1
1	D	244	LEU	4.9
1	C	245	LYS	4.8
1	D	92	GLY	4.8
1	C	186	PRO	4.7
2	E	499	GLY	4.5
1	C	231	ASP	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	183	SER	4.4
1	C	187	THR	4.3
1	D	44	GLY	4.2
2	E	498	ARG	4.1
1	B	244	LEU	4.1
2	H	510	ASN	4.1
1	A	184	LYS	3.9
1	B	187	THR	3.9
1	C	232	ALA	3.9
1	A	189	GLN	3.9
1	C	178	LEU	3.8
2	G	498	ARG	3.8
1	D	47	ARG	3.7
1	D	185	ASP	3.7
1	A	47	ARG	3.4
1	C	183	SER	3.4
1	A	190	LYS	3.3
1	D	171	PHE	3.2
2	F	498	ARG	3.2
1	D	91	LEU	3.1
1	A	182	MET	3.0
1	A	245	LYS	3.0
1	B	188	THR	3.0
1	C	230	ASP	3.0
1	A	193	ASN	2.9
2	G	509	VAL	2.9
1	C	174	ALA	2.9
1	C	95	HIS	2.8
1	D	95	HIS	2.8
1	C	244	LEU	2.8
1	D	183	SER	2.8
1	A	45	GLU	2.7
1	D	93	LYS	2.7
1	D	122	MET	2.7
2	E	510	ASN	2.6
1	C	179	LYS	2.6
1	B	186	PRO	2.6
1	A	187	THR	2.5
1	D	184	LYS	2.5
1	A	204	LEU	2.5
1	C	44	GLY	2.5
1	A	200	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	229	LEU	2.4
1	B	199	ILE	2.4
1	B	92	GLY	2.3
1	C	176	LYS	2.3
1	A	44	GLY	2.3
1	A	122	MET	2.3
1	D	45	GLU	2.3
2	G	499	GLY	2.3
1	A	244	LEU	2.2
1	B	47	ARG	2.2
1	D	46	ALA	2.2
2	G	497	PHE	2.2
2	H	502	LEU	2.2
1	B	93	LYS	2.1
1	C	100	LEU	2.1
2	G	496	GLU	2.1
1	A	208	VAL	2.1
1	D	211	ASN	2.1
1	C	235	TYR	2.1
2	F	509	VAL	2.0
1	C	200	ARG	2.0
1	C	93	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.