



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 11:09 pm GMT

PDB ID : 3ZC1  
Title : Crystal structure of AfC3PO  
Authors : Parizotto, E.A.; Lowe, E.D.; Parker, J.S.  
Deposited on : 2012-11-14  
Resolution : 3.27 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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

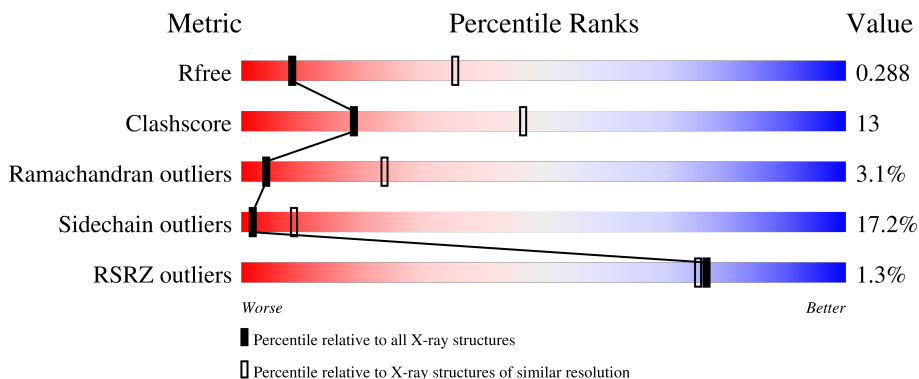
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.27 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))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	199	 64% 24% 7% 5%
1	B	199	 2% 56% 33% 6% 5%
1	C	199	 58% 30% 7% 5%
1	D	199	 2% 54% 33% 8% 6%
1	E	199	 55% 31% 10% 5%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	199	<p>%</p> <p>56% 32% 7% • 5%</p>
1	G	199	<p>%</p> <p>56% 33% 6% • 5%</p>
1	H	199	<p>3%</p> <p>59% 29% 6% 6%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11820 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 AFTRAX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	190	1487	950	250	279	8	0	0	0
1	B	190	1495	950	255	282	8	0	0	0
1	C	189	1478	939	249	283	7	0	0	0
1	D	187	1479	943	249	280	7	0	0	0
1	E	190	1494	955	255	276	8	0	0	0
1	F	190	1486	948	251	279	8	0	0	0
1	G	189	1451	920	244	279	8	0	0	0
1	H	187	1437	911	245	273	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O28024
A	-1	PRO	-	expression tag	UNP O28024
A	0	HIS	-	expression tag	UNP O28024
B	-2	GLY	-	expression tag	UNP O28024
B	-1	PRO	-	expression tag	UNP O28024
B	0	HIS	-	expression tag	UNP O28024
C	-2	GLY	-	expression tag	UNP O28024
C	-1	PRO	-	expression tag	UNP O28024
C	0	HIS	-	expression tag	UNP O28024
D	-2	GLY	-	expression tag	UNP O28024
D	-1	PRO	-	expression tag	UNP O28024
D	0	HIS	-	expression tag	UNP O28024
E	-2	GLY	-	expression tag	UNP O28024

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP O28024
E	0	HIS	-	expression tag	UNP O28024
F	-2	GLY	-	expression tag	UNP O28024
F	-1	PRO	-	expression tag	UNP O28024
F	0	HIS	-	expression tag	UNP O28024
G	-2	GLY	-	expression tag	UNP O28024
G	-1	PRO	-	expression tag	UNP O28024
G	0	HIS	-	expression tag	UNP O28024
H	-2	GLY	-	expression tag	UNP O28024
H	-1	PRO	-	expression tag	UNP O28024
H	0	HIS	-	expression tag	UNP O28024

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0

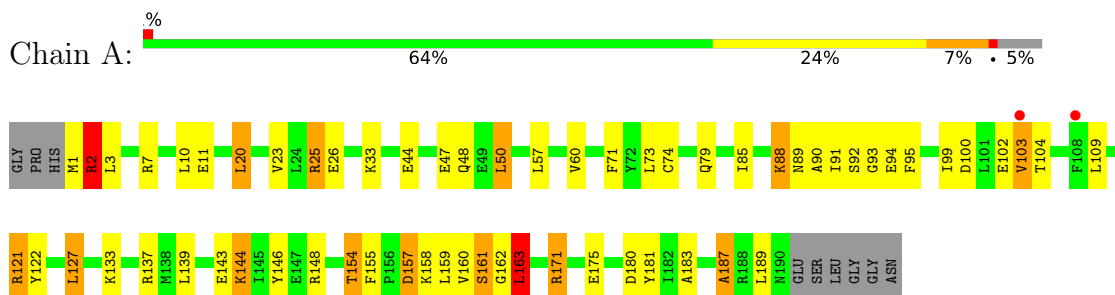
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total O 3 3	0	0
3	D	1	Total O 1 1	0	0
3	F	3	Total O 3 3	0	0
3	G	1	Total O 1 1	0	0

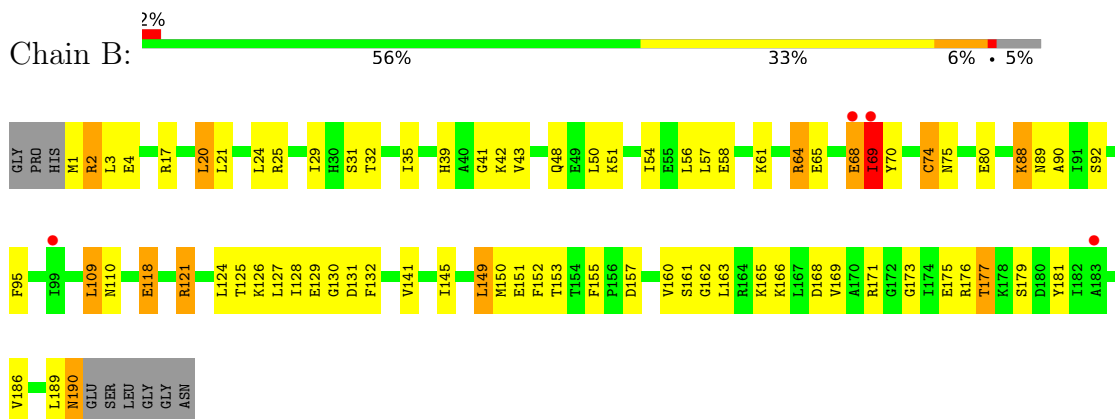
### 3 Residue-property plots [i](#)

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.

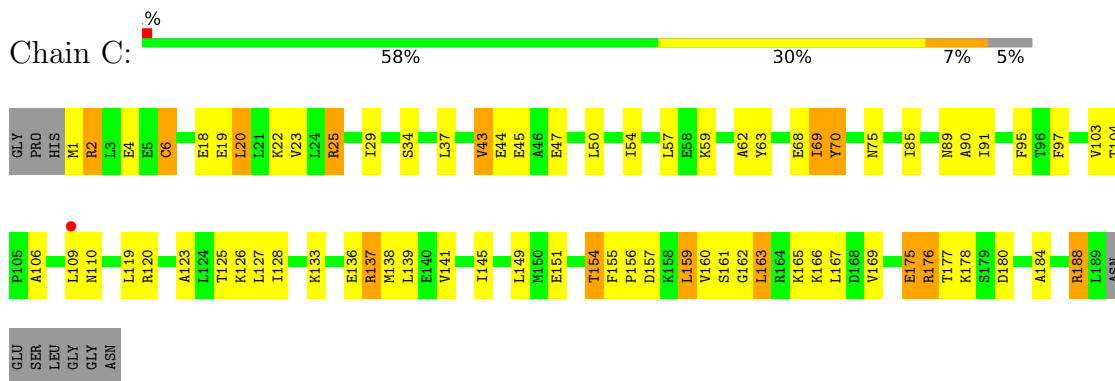
- Molecule 1: AFTRAX



- Molecule 1: AFTRAX



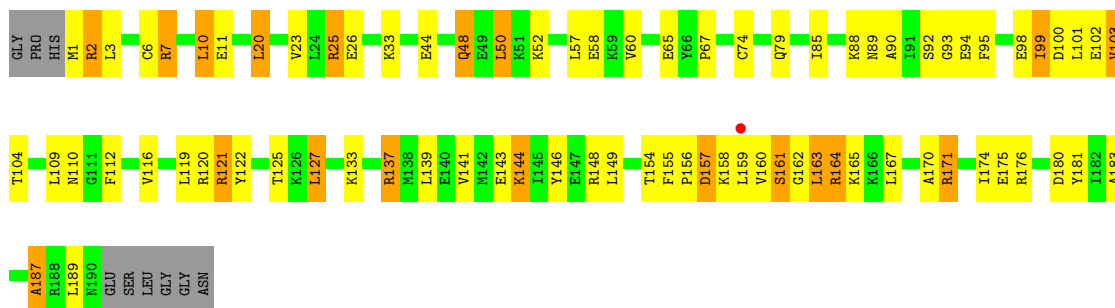
- Molecule 1: AFTRAX



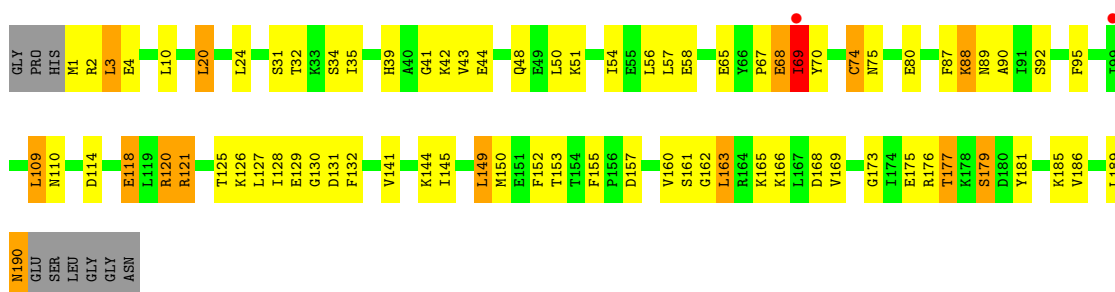
- Molecule 1: AFTRAX



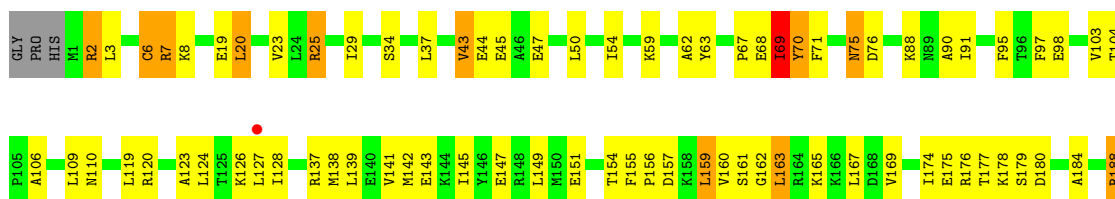
- Molecule 1: AFTRAX



- Molecule 1: AFTRAX



- Molecule 1: AFTRAX



L189  
 ASN  
 GLU  
 SER  
 LEU  
 GLY  
 ASN

• Molecule 1: AFTRAX

Chain H:  3% 59% 29% 6% 6%

GLY  
 PRO  
 HIS  
 M1  
 R2  
 R7  
 L10  
 E14  
 E19  
 L20  
 L21  
 K22  
 V23  
 L24  
 R25  
 H30  
 S31  
 S34  
 I35  
 H39  
 V43  
 E44  
 L50  
 K51  
 K52  
 L56  
 L57  
 K61  
 A62  
 Y63  
 I69  
 M78  
 Q79  
 E80  
 I85  
 S92  
 G93  
 E94  
 F97  
 E102  
 V103  
 T104

F108  
 L109  
 M110  
 G111  
 F112  
 A113  
 D114  
 A115  
 V116  
 G117  
 E118  
 L119  
 R120  
 R121  
 K126  
 L127  
 I128  
 D131  
 S134  
 R137  
 M138  
 L139  
 E140  
 V141  
 Y146  
 F147  
 R148  
 L149  
 M150  
 E151  
 F152  
 T153  
 T154  
 S161  
 G162  
 L163  
 R164  
 K165  
 K166  
 L167  
 D168  
 V169  
 A170  
 R171  
 G172  
 G173  
 I174  
 E175  
 R176  
 T177  
 K178  
 S179  
 D180  
 Y181

I182  
 A183  
 A184  
 K185  
 V186  
 A187  
 ARG  
 LEU  
 ASN  
 GLU  
 SER  
 LEU  
 GLY  
 ASN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.31Å 183.31Å 111.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.56 – 3.27 70.75 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.56-3.27) 98.1 (70.75-3.27)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 3.26Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.221 , 0.281 0.226 , 0.288	Depositor DCC
$R_{free}$ test set	2000 reflections (6.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.8	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 72.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.04% 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: MG

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	0.49	0/1506	0.63	0/2025
1	B	0.48	0/1515	0.65	0/2038
1	C	0.49	0/1497	0.66	0/2016
1	D	0.47	0/1499	0.62	1/2016 (0.0%)
1	E	0.50	1/1513 (0.1%)	0.63	0/2031
1	F	0.50	0/1505	0.65	0/2024
1	G	0.49	0/1470	0.66	0/1983
1	H	0.48	0/1456	0.63	1/1963 (0.1%)
All	All	0.49	1/11961 (0.0%)	0.64	2/16096 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	6	CYS	CB-SG	5.27	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	LEU	CA-CB-CG	5.68	128.36	115.30
1	H	57	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1487	0	1485	33	0
1	B	1495	0	1479	45	0
1	C	1478	0	1454	47	0
1	D	1479	0	1475	48	0
1	E	1494	0	1513	48	0
1	F	1486	0	1486	46	0
1	G	1451	0	1395	48	0
1	H	1437	0	1387	33	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
All	All	11820	0	11674	309	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 13.

All (309) 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:G:2:ARG:NH1	1:G:6:CYS:SG	2.50	0.85
1:C:2:ARG:NH1	1:C:6:CYS:SG	2.54	0.80
1:F:161:SER:OG	1:F:162:GLY:N	2.20	0.74
1:D:183:ALA:O	1:D:185:LYS:N	2.22	0.72
1:H:183:ALA:O	1:H:185:LYS:N	2.22	0.72
1:C:156:PRO:HG2	1:C:159:LEU:HB2	1.71	0.71
1:E:109:LEU:HB3	1:E:163:LEU:HD21	1.72	0.71
1:A:157:ASP:O	1:A:159:LEU:N	2.23	0.71
1:C:180:ASP:OD2	1:D:179:SER:OG	2.08	0.70
1:F:90:ALA:HA	1:F:95:PHE:HB2	1.73	0.70
1:B:161:SER:OG	1:B:162:GLY:N	2.25	0.70
1:G:156:PRO:HG2	1:G:159:LEU:HB2	1.73	0.70
1:B:25:ARG:NH2	1:H:14:GLU:OE2	2.24	0.69
1:B:90:ALA:HA	1:B:95:PHE:HB2	1.74	0.69
1:C:68:GLU:O	1:C:69:ILE:HG12	1.93	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:O	1:A:94:GLU:N	2.22	0.69
1:B:125:THR:HG22	1:C:178:LYS:NZ	2.09	0.68
1:A:180:ASP:OD1	1:B:176:ARG:NH2	2.25	0.68
1:E:157:ASP:O	1:E:159:LEU:N	2.27	0.67
1:A:161:SER:OG	1:A:162:GLY:N	2.28	0.66
1:E:144:LYS:HE3	1:E:148:ARG:HG2	1.78	0.66
1:E:160:VAL:HG13	1:E:163:LEU:HB2	1.77	0.66
1:B:41:GLY:O	1:B:43:VAL:N	2.29	0.65
1:B:121:ARG:O	1:B:125:THR:HG23	1.96	0.65
1:C:161:SER:OG	1:C:162:GLY:N	2.28	0.65
1:G:68:GLU:O	1:G:69:ILE:HG12	1.95	0.65
1:E:92:SER:O	1:E:94:GLU:N	2.23	0.65
1:B:50:LEU:O	1:B:54:ILE:HG13	1.97	0.65
1:E:183:ALA:O	1:F:179:SER:OG	2.15	0.65
1:A:160:VAL:HG13	1:A:163:LEU:HB2	1.79	0.64
1:E:161:SER:OG	1:E:162:GLY:N	2.30	0.64
1:F:130:GLY:O	1:F:132:PHE:N	2.31	0.64
1:G:106:ALA:O	1:G:110:ASN:ND2	2.31	0.64
1:D:8:LYS:O	1:D:12:GLU:HG3	1.99	0.63
1:A:155:PHE:HA	1:D:25:ARG:HH21	1.63	0.63
1:B:130:GLY:O	1:B:132:PHE:N	2.32	0.62
1:A:144:LYS:HE3	1:A:148:ARG:HG2	1.81	0.62
1:C:106:ALA:O	1:C:110:ASN:ND2	2.32	0.62
1:H:161:SER:OG	1:H:162:GLY:N	2.32	0.62
1:C:155:PHE:CE2	1:H:10:LEU:HB3	2.35	0.61
1:F:41:GLY:O	1:F:43:VAL:N	2.32	0.61
1:G:157:ASP:HA	1:G:160:VAL:HG12	1.82	0.61
1:B:145:ILE:O	1:B:149:LEU:HB2	2.00	0.61
1:F:132:PHE:HE2	1:F:185:LYS:HG3	1.65	0.61
1:A:102:GLU:HA	1:A:103:VAL:HB	1.82	0.61
1:D:39:HIS:CE1	1:D:121:ARG:HG2	2.36	0.61
1:F:121:ARG:O	1:F:125:THR:HG23	2.01	0.60
1:B:70:TYR:O	1:B:74:CYS:HB2	2.00	0.60
1:G:7:ARG:HG3	1:G:8:LYS:N	2.16	0.60
1:F:70:TYR:O	1:F:74:CYS:HB2	2.02	0.60
1:E:102:GLU:HA	1:E:103:VAL:HB	1.84	0.60
1:B:29:ILE:HG12	1:C:154:THR:HB	1.82	0.59
1:A:90:ALA:HA	1:A:95:PHE:HB2	1.84	0.59
1:F:20:LEU:HD22	1:F:24:LEU:HG	1.83	0.59
1:A:92:SER:O	1:A:94:GLU:HG2	2.02	0.59
1:A:121:ARG:NH2	1:B:168:ASP:OD2	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD22	1:B:24:LEU:HG	1.84	0.59
1:F:127:LEU:HD21	1:F:181:TYR:HA	1.85	0.59
1:D:71:PHE:CE2	1:G:67:PRO:HB2	2.38	0.59
1:C:157:ASP:HA	1:C:160:VAL:HG12	1.84	0.58
1:H:79:GLN:NE2	1:H:110:ASN:HB3	2.18	0.58
1:E:164:ARG:NH1	1:E:164:ARG:HB2	2.18	0.58
1:G:120:ARG:HG3	1:G:120:ARG:HH11	1.68	0.58
1:F:130:GLY:O	1:F:132:PHE:HD1	1.87	0.58
1:B:127:LEU:HD21	1:B:181:TYR:HA	1.84	0.58
1:E:143:GLU:OE2	1:E:171:ARG:NH2	2.31	0.58
1:B:61:LYS:O	1:B:64:ARG:HG3	2.04	0.57
1:D:67:PRO:HB3	1:G:67:PRO:HB3	1.86	0.57
1:D:79:GLN:NE2	1:D:110:ASN:HB3	2.19	0.57
1:G:161:SER:OG	1:G:162:GLY:N	2.36	0.57
1:G:25:ARG:O	1:G:29:ILE:HG13	2.04	0.57
1:E:90:ALA:HA	1:E:95:PHE:HB2	1.86	0.57
1:G:50:LEU:O	1:G:54:ILE:HG12	2.05	0.57
1:H:92:SER:O	1:H:94:GLU:N	2.35	0.57
1:F:190:ASN:N	1:F:190:ASN:OD1	2.38	0.57
1:H:39:HIS:CE1	1:H:121:ARG:HG2	2.39	0.57
1:D:92:SER:O	1:D:94:GLU:N	2.37	0.56
1:B:125:THR:HG22	1:C:178:LYS:HZ2	1.69	0.56
1:B:130:GLY:O	1:B:132:PHE:HD1	1.89	0.56
1:C:29:ILE:HG12	1:D:154:THR:HG21	1.88	0.56
1:A:143:GLU:OE2	1:A:171:ARG:NH2	2.32	0.56
1:F:50:LEU:O	1:F:54:ILE:HG13	2.04	0.56
1:G:90:ALA:HA	1:G:95:PHE:HB2	1.87	0.56
1:B:88:LYS:NZ	1:B:92:SER:OG	2.39	0.56
1:E:44:GLU:OE1	1:E:44:GLU:N	2.32	0.56
1:H:173:GLY:O	1:H:177:THR:OG1	2.24	0.56
1:B:190:ASN:OD1	1:B:190:ASN:N	2.39	0.55
1:G:29:ILE:HG12	1:H:154:THR:HG21	1.88	0.55
1:G:37:LEU:HD13	1:G:45:GLU:HB2	1.88	0.55
1:H:146:TYR:CE1	1:H:171:ARG:HG2	2.41	0.55
1:A:127:LEU:HD21	1:A:181:TYR:HA	1.88	0.55
1:D:127:LEU:HD21	1:D:181:TYR:HB2	1.88	0.55
1:C:137:ARG:HB2	1:C:137:ARG:CZ	2.37	0.55
1:G:137:ARG:HB2	1:G:137:ARG:CZ	2.37	0.55
1:C:90:ALA:HA	1:C:95:PHE:HB2	1.89	0.54
1:C:119:LEU:HD13	1:C:141:VAL:HG13	1.90	0.54
1:G:180:ASP:OD2	1:H:179:SER:OG	2.24	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:TYR:CE1	1:D:171:ARG:HG2	2.42	0.54
1:D:161:SER:OG	1:D:162:GLY:N	2.38	0.54
1:F:88:LYS:NZ	1:F:92:SER:OG	2.41	0.53
1:H:127:LEU:HD21	1:H:181:TYR:HB2	1.90	0.53
1:H:79:GLN:HE22	1:H:110:ASN:HB3	1.74	0.53
1:C:37:LEU:HD13	1:C:45:GLU:HB2	1.91	0.53
1:F:173:GLY:O	1:F:177:THR:OG1	2.24	0.53
1:B:109:LEU:HD21	1:B:152:PHE:CD2	2.44	0.53
1:F:145:ILE:O	1:F:149:LEU:HB2	2.08	0.53
1:G:43:VAL:O	1:G:47:GLU:HG3	2.08	0.53
1:A:89:ASN:HB3	1:A:95:PHE:HA	1.91	0.53
1:D:78:MET:SD	1:D:103:VAL:HG13	2.49	0.53
1:G:25:ARG:NH1	1:H:154:THR:O	2.42	0.53
1:A:23:VAL:HG12	1:A:60:VAL:HG23	1.90	0.52
1:A:183:ALA:O	1:B:179:SER:OG	2.19	0.52
1:C:50:LEU:O	1:C:54:ILE:HG12	2.10	0.52
1:C:165:LYS:O	1:C:169:VAL:HG23	2.10	0.52
1:E:23:VAL:HG12	1:E:60:VAL:HG23	1.91	0.52
1:E:127:LEU:HD21	1:E:181:TYR:HA	1.90	0.52
1:E:146:TYR:CZ	1:E:171:ARG:HG2	2.45	0.52
1:D:49:GLU:HA	1:D:52:LYS:HD3	1.91	0.51
1:E:89:ASN:HB3	1:E:95:PHE:HA	1.92	0.51
1:A:44:GLU:OE1	1:A:44:GLU:N	2.35	0.51
1:A:187:ALA:HA	1:A:189:LEU:N	2.25	0.51
1:G:119:LEU:HD13	1:G:141:VAL:HG13	1.93	0.51
1:D:97:PHE:CD2	1:G:3:LEU:HD11	2.45	0.51
1:G:165:LYS:O	1:G:169:VAL:HG23	2.10	0.51
1:A:1:MET:O	1:A:3:LEU:N	2.44	0.51
1:D:28:ARG:HH21	1:D:77:ALA:HB2	1.76	0.51
1:A:146:TYR:CZ	1:A:171:ARG:HG2	2.45	0.50
1:A:189:LEU:H	1:A:189:LEU:HD22	1.76	0.50
1:E:187:ALA:HA	1:E:189:LEU:N	2.26	0.50
1:D:79:GLN:HE22	1:D:110:ASN:HB3	1.77	0.50
1:C:184:ALA:O	1:C:188:ARG:HD2	2.11	0.50
1:G:44:GLU:HA	1:G:47:GLU:CD	2.32	0.50
1:A:109:LEU:HB3	1:A:163:LEU:HD21	1.93	0.50
1:B:2:ARG:HG3	1:E:98:GLU:HA	1.93	0.50
1:D:173:GLY:O	1:D:177:THR:OG1	2.29	0.50
1:A:146:TYR:CE1	1:A:171:ARG:HG2	2.47	0.50
1:D:48:GLN:O	1:D:52:LYS:HD2	2.12	0.50
1:F:39:HIS:NE2	1:F:118:GLU:HG3	2.27	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:O	1:C:29:ILE:HG13	2.11	0.50
1:F:109:LEU:HD21	1:F:152:PHE:CD2	2.46	0.50
1:E:110:ASN:OD1	1:E:163:LEU:HD23	2.12	0.49
1:F:110:ASN:HB3	1:F:166:LYS:HE2	1.94	0.49
1:H:39:HIS:NE2	1:H:118:GLU:HG3	2.27	0.49
1:B:126:LYS:O	1:B:129:GLU:N	2.45	0.49
1:C:120:ARG:HG3	1:C:120:ARG:HH11	1.77	0.49
1:E:180:ASP:OD1	1:F:176:ARG:NH2	2.42	0.49
1:G:20:LEU:HD23	1:G:63:TYR:HD2	1.77	0.49
1:E:154:THR:OG1	1:E:155:PHE:N	2.45	0.49
1:D:126:LYS:HB3	1:D:131:ASP:HB3	1.94	0.49
1:F:132:PHE:CE2	1:F:185:LYS:HG3	2.47	0.49
1:F:1:MET:O	1:F:3:LEU:N	2.46	0.48
1:F:176:ARG:O	1:F:179:SER:HB2	2.13	0.48
1:G:139:LEU:HD22	1:G:177:THR:HG22	1.95	0.48
1:B:110:ASN:HB3	1:B:166:LYS:HE2	1.95	0.48
1:A:154:THR:OG1	1:A:155:PHE:N	2.46	0.48
1:E:116:VAL:HG11	1:E:170:ALA:HB1	1.95	0.48
1:F:1:MET:O	1:F:4:GLU:N	2.38	0.48
1:B:1:MET:O	1:B:3:LEU:N	2.46	0.48
1:D:39:HIS:NE2	1:D:118:GLU:HG3	2.29	0.48
1:D:101:LEU:HB3	1:D:103:VAL:HG23	1.95	0.48
1:E:121:ARG:NH2	1:F:168:ASP:OD2	2.39	0.48
1:G:69:ILE:HG13	1:G:70:TYR:H	1.79	0.48
1:B:39:HIS:NE2	1:B:118:GLU:HG3	2.29	0.47
1:F:150:MET:O	1:F:153:THR:HG22	2.14	0.47
1:G:184:ALA:O	1:G:188:ARG:HD2	2.14	0.47
1:E:120:ARG:HH22	1:E:176:ARG:NH2	2.11	0.47
1:H:120:ARG:HD2	1:H:173:GLY:O	2.13	0.47
1:C:25:ARG:NH1	1:D:154:THR:O	2.47	0.47
1:A:71:PHE:CE2	1:F:67:PRO:HB2	2.48	0.47
1:D:98:GLU:OE1	1:G:2:ARG:N	2.31	0.47
1:G:97:PHE:HZ	1:G:145:ILE:HA	1.78	0.47
1:G:142:MET:HE1	1:G:174:ILE:HA	1.96	0.47
1:A:50:LEU:HD21	1:A:85:ILE:HG13	1.96	0.47
1:H:78:MET:SD	1:H:103:VAL:HG13	2.54	0.47
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.66	0.47
1:B:31:SER:O	1:B:35:ILE:HG13	2.14	0.47
1:G:2:ARG:HD2	1:G:2:ARG:O	2.14	0.47
1:B:165:LYS:O	1:B:169:VAL:HG23	2.15	0.47
1:C:69:ILE:HG13	1:C:70:TYR:H	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.65	0.46
1:C:59:LYS:O	1:C:62:ALA:HB3	2.15	0.46
1:G:123:ALA:O	1:G:127:LEU:HB2	2.15	0.46
1:C:43:VAL:O	1:C:47:GLU:HG3	2.16	0.46
1:G:163:LEU:HD22	1:G:167:LEU:HG	1.96	0.46
1:C:44:GLU:HA	1:C:47:GLU:CD	2.35	0.46
1:D:150:MET:HG2	1:D:167:LEU:HD13	1.98	0.46
1:H:126:LYS:HB3	1:H:131:ASP:HB3	1.97	0.46
1:H:171:ARG:NH1	1:H:175:GLU:OE1	2.48	0.46
1:C:19:GLU:O	1:C:23:VAL:HG23	2.16	0.46
1:D:71:PHE:HE2	1:G:67:PRO:HB2	1.79	0.46
1:B:125:THR:HG22	1:C:178:LYS:HZ3	1.79	0.46
1:B:173:GLY:O	1:B:177:THR:OG1	2.34	0.46
1:C:163:LEU:HD22	1:C:167:LEU:HG	1.97	0.45
1:E:189:LEU:H	1:E:189:LEU:HD22	1.80	0.45
1:F:165:LYS:O	1:F:169:VAL:HG23	2.16	0.45
1:D:19:GLU:O	1:D:23:VAL:HG23	2.16	0.45
1:A:47:GLU:OE1	1:A:88:LYS:HE2	2.17	0.45
1:F:189:LEU:HB2	1:F:190:ASN:OD1	2.17	0.45
1:F:89:ASN:HB3	1:F:95:PHE:HA	1.99	0.45
1:F:126:LYS:O	1:F:129:GLU:N	2.50	0.45
1:E:164:ARG:HB2	1:E:164:ARG:HH11	1.80	0.45
1:F:144:LYS:HB2	1:F:144:LYS:HE3	1.72	0.45
1:F:157:ASP:O	1:F:161:SER:N	2.41	0.45
1:H:19:GLU:O	1:H:23:VAL:HG23	2.16	0.45
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.84	0.45
1:D:67:PRO:HB2	1:G:71:PHE:CE2	2.52	0.45
1:D:171:ARG:NH1	1:D:175:GLU:OE1	2.50	0.45
1:H:150:MET:HG2	1:H:167:LEU:HD13	1.99	0.45
1:E:48:GLN:O	1:E:52:LYS:HG3	2.17	0.45
1:B:155:PHE:HZ	1:E:11:GLU:HG3	1.82	0.45
1:E:1:MET:O	1:E:3:LEU:N	2.50	0.45
1:E:65:GLU:O	1:E:67:PRO:HD3	2.17	0.45
1:D:116:VAL:HG11	1:D:170:ALA:HB1	1.99	0.44
1:E:155:PHE:HA	1:H:25:ARG:HH21	1.82	0.44
1:B:89:ASN:HB3	1:B:95:PHE:HA	1.99	0.44
1:B:150:MET:O	1:B:153:THR:HG22	2.18	0.44
1:C:2:ARG:HD2	1:C:2:ARG:O	2.18	0.44
1:C:20:LEU:HD23	1:C:63:TYR:HD2	1.83	0.44
1:D:28:ARG:NH2	1:D:77:ALA:HB2	2.33	0.44
1:G:59:LYS:O	1:G:62:ALA:HB3	2.17	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LEU:HD13	1:C:85:ILE:HG12	1.98	0.44
1:C:139:LEU:HD22	1:C:177:THR:HG22	1.99	0.44
1:D:165:LYS:O	1:D:169:VAL:HG23	2.18	0.44
1:H:92:SER:C	1:H:94:GLU:H	2.19	0.44
1:B:48:GLN:O	1:B:51:LYS:HB3	2.16	0.44
1:B:68:GLU:O	1:B:69:ILE:HG12	2.17	0.44
1:G:91:ILE:HA	1:G:138:MET:HE3	2.00	0.44
1:H:110:ASN:O	1:H:114:ASP:HB2	2.17	0.44
1:C:91:ILE:HA	1:C:138:MET:HE3	2.00	0.44
1:D:1:MET:O	1:D:3:LEU:N	2.51	0.44
1:E:146:TYR:CE1	1:E:171:ARG:HG2	2.53	0.44
1:E:156:PRO:HD2	1:E:159:LEU:HD12	2.00	0.43
1:A:11:GLU:HG3	1:F:155:PHE:CZ	2.54	0.43
1:D:120:ARG:HD2	1:D:173:GLY:O	2.18	0.43
1:E:25:ARG:HG3	1:E:26:GLU:N	2.32	0.43
1:F:125:THR:HG22	1:G:178:LYS:NZ	2.33	0.43
1:B:155:PHE:CZ	1:E:11:GLU:HG3	2.53	0.43
1:E:50:LEU:HD21	1:E:85:ILE:HG13	1.99	0.43
1:E:99:ILE:O	1:E:101:LEU:N	2.43	0.43
1:E:170:ALA:O	1:E:174:ILE:HG13	2.18	0.43
1:D:10:LEU:HB3	1:G:155:PHE:CE2	2.53	0.43
1:F:114:ASP:OD1	1:F:166:LYS:HE3	2.18	0.43
1:C:89:ASN:HB3	1:C:95:PHE:HA	2.00	0.43
1:H:137:ARG:O	1:H:140:GLU:HB2	2.19	0.43
1:E:165:LYS:H	1:E:165:LYS:HG2	1.67	0.43
1:G:88:LYS:O	1:G:91:ILE:HG13	2.18	0.43
1:C:133:LYS:O	1:C:136:GLU:HG2	2.19	0.43
1:G:119:LEU:HD22	1:G:138:MET:SD	2.59	0.43
1:G:143:GLU:O	1:G:147:GLU:HG3	2.19	0.43
1:B:1:MET:O	1:B:4:GLU:N	2.38	0.42
1:C:18:GLU:O	1:C:22:LYS:HG3	2.19	0.42
1:C:123:ALA:O	1:C:127:LEU:HB2	2.17	0.42
1:D:163:LEU:HD22	1:D:167:LEU:HG	2.01	0.42
1:D:166:LYS:HE3	1:D:166:LYS:HB3	1.93	0.42
1:F:50:LEU:HD23	1:F:50:LEU:HA	1.85	0.42
1:H:30:HIS:CE1	1:H:52:LYS:HB3	2.54	0.42
1:H:146:TYR:CZ	1:H:171:ARG:HG2	2.54	0.42
1:C:2:ARG:CZ	1:C:6:CYS:SG	3.07	0.42
1:D:146:TYR:CZ	1:D:171:ARG:HG2	2.54	0.42
1:C:139:LEU:HD21	1:C:178:LYS:HG2	2.02	0.42
1:D:20:LEU:HD21	1:D:60:VAL:HG13	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:LEU:HD22	1:H:24:LEU:HG	2.01	0.42
1:H:116:VAL:HG11	1:H:170:ALA:HB1	2.01	0.42
1:A:25:ARG:HG3	1:A:26:GLU:N	2.34	0.42
1:B:189:LEU:HB2	1:B:190:ASN:OD1	2.20	0.42
1:C:119:LEU:HD22	1:C:138:MET:SD	2.59	0.42
1:E:20:LEU:HD23	1:E:20:LEU:HA	1.84	0.42
1:F:165:LYS:O	1:F:168:ASP:HB2	2.20	0.42
1:D:167:LEU:HD23	1:D:167:LEU:HA	1.87	0.42
1:F:3:LEU:HD22	1:F:3:LEU:HA	1.81	0.42
1:C:125:THR:HG22	1:D:178:LYS:NZ	2.34	0.42
1:E:10:LEU:HD12	1:E:10:LEU:HA	1.86	0.42
1:F:149:LEU:HD12	1:F:149:LEU:HA	1.62	0.42
1:H:126:LYS:HD3	1:H:126:LYS:HA	1.88	0.42
1:A:160:VAL:CG1	1:A:163:LEU:HB2	2.47	0.41
1:F:68:GLU:O	1:F:69:ILE:HG12	2.20	0.41
1:D:2:ARG:HB2	1:G:98:GLU:OE1	2.20	0.41
1:E:137:ARG:HB2	1:E:137:ARG:CZ	2.50	0.41
1:H:165:LYS:O	1:H:169:VAL:HG23	2.20	0.41
1:A:91:ILE:HG22	1:A:122:TYR:CD2	2.55	0.41
1:C:176:ARG:HH12	1:D:176:ARG:HG2	1.86	0.41
1:D:22:LYS:HA	1:D:22:LYS:HD3	1.75	0.41
1:E:119:LEU:HD13	1:E:141:VAL:HG13	2.02	0.41
1:F:163:LEU:HD23	1:F:163:LEU:HA	1.88	0.41
1:G:19:GLU:O	1:G:23:VAL:HG23	2.20	0.41
1:G:139:LEU:HD21	1:G:178:LYS:HG2	2.02	0.41
1:B:124:LEU:HD23	1:C:175:GLU:HG3	2.02	0.41
1:B:157:ASP:O	1:B:161:SER:N	2.41	0.41
1:C:57:LEU:HD13	1:C:57:LEU:O	2.20	0.41
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.87	0.41
1:C:97:PHE:HZ	1:C:145:ILE:HA	1.86	0.41
1:E:120:ARG:NH2	1:E:176:ARG:NH2	2.69	0.41
1:F:35:ILE:HG23	1:F:87:PHE:CD2	2.56	0.41
1:G:124:LEU:HD12	1:G:124:LEU:HA	1.92	0.41
1:B:168:ASP:HA	1:B:171:ARG:NH1	2.35	0.41
1:C:1:MET:O	1:C:4:GLU:N	2.54	0.41
1:D:156:PRO:HB2	1:D:159:LEU:HD21	2.03	0.41
1:B:151:GLU:O	1:E:7:ARG:NH2	2.54	0.41
1:E:149:LEU:HD23	1:E:167:LEU:HD21	2.02	0.41
1:F:120:ARG:NH2	1:G:179:SER:OG	2.53	0.41
1:E:99:ILE:HD11	1:E:112:PHE:CE1	2.56	0.40
1:E:122:TYR:HA	1:E:125:THR:HG22	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:O	1:B:21:LEU:HG	2.22	0.40
1:H:167:LEU:HD23	1:H:167:LEU:HA	1.88	0.40
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.90	0.40
1:F:48:GLN:O	1:F:51:LYS:HB3	2.21	0.40
1:H:163:LEU:HD22	1:H:167:LEU:HG	2.04	0.40
1:F:31:SER:O	1:F:34:SER:HB3	2.21	0.40
1:G:143:GLU:OE2	1:G:178:LYS:NZ	2.47	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	188/199 (94%)	164 (87%)	15 (8%)	9 (5%)	2	14
1	B	188/199 (94%)	159 (85%)	25 (13%)	4 (2%)	7	32
1	C	187/199 (94%)	160 (86%)	23 (12%)	4 (2%)	7	32
1	D	185/199 (93%)	152 (82%)	29 (16%)	4 (2%)	6	31
1	E	188/199 (94%)	164 (87%)	16 (8%)	8 (4%)	2	16
1	F	188/199 (94%)	164 (87%)	20 (11%)	4 (2%)	7	32
1	G	187/199 (94%)	159 (85%)	23 (12%)	5 (3%)	5	26
1	H	185/199 (93%)	147 (80%)	30 (16%)	8 (4%)	2	16
All	All	1496/1592 (94%)	1269 (85%)	181 (12%)	46 (3%)	4	24

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	B	2	ARG
1	B	42	LYS

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	131	ASP
1	E	2	ARG
1	F	2	ARG
1	F	42	LYS
1	F	131	ASP
1	A	93	GLY
1	A	157	ASP
1	A	158	LYS
1	C	69	ILE
1	D	2	ARG
1	E	93	GLY
1	E	157	ASP
1	E	158	LYS
1	G	69	ILE
1	G	151	GLU
1	H	2	ARG
1	A	100	ASP
1	A	163	LEU
1	A	187	ALA
1	C	70	TYR
1	D	69	ILE
1	D	93	GLY
1	D	131	ASP
1	E	187	ALA
1	G	70	TYR
1	H	69	ILE
1	E	100	ASP
1	E	103	VAL
1	E	161	SER
1	H	63	TYR
1	H	93	GLY
1	H	131	ASP
1	A	103	VAL
1	A	161	SER
1	C	75	ASN
1	C	151	GLU
1	H	61	LYS
1	H	102	GLU
1	H	134	SER
1	G	75	ASN
1	G	76	ASP
1	B	69	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	69	ILE

### 5.3.2 Protein sidechains [i](#)

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	148/167 (89%)	123 (83%)	25 (17%)	2 9
1	B	149/167 (89%)	124 (83%)	25 (17%)	2 9
1	C	147/167 (88%)	127 (86%)	20 (14%)	3 16
1	D	149/167 (89%)	120 (80%)	29 (20%)	1 5
1	E	150/167 (90%)	125 (83%)	25 (17%)	2 9
1	F	149/167 (89%)	120 (80%)	29 (20%)	1 5
1	G	140/167 (84%)	119 (85%)	21 (15%)	3 12
1	H	138/167 (83%)	111 (80%)	27 (20%)	1 5
All	All	1170/1336 (88%)	969 (83%)	201 (17%)	2 9

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	7	ARG
1	A	10	LEU
1	A	20	LEU
1	A	25	ARG
1	A	33	LYS
1	A	48	GLN
1	A	50	LEU
1	A	57	LEU
1	A	73	LEU
1	A	74	CYS
1	A	79	GLN
1	A	88	LYS
1	A	99	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	104	THR
1	A	121	ARG
1	A	127	LEU
1	A	133	LYS
1	A	137	ARG
1	A	139	LEU
1	A	144	LYS
1	A	154	THR
1	A	163	LEU
1	A	171	ARG
1	A	175	GLU
1	B	20	LEU
1	B	32	THR
1	B	56	LEU
1	B	57	LEU
1	B	58	GLU
1	B	64	ARG
1	B	65	GLU
1	B	68	GLU
1	B	69	ILE
1	B	74	CYS
1	B	75	ASN
1	B	80	GLU
1	B	88	LYS
1	B	109	LEU
1	B	118	GLU
1	B	121	ARG
1	B	128	ILE
1	B	141	VAL
1	B	149	LEU
1	B	160	VAL
1	B	163	LEU
1	B	175	GLU
1	B	177	THR
1	B	186	VAL
1	B	190	ASN
1	C	2	ARG
1	C	6	CYS
1	C	20	LEU
1	C	25	ARG
1	C	34	SER
1	C	43	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	103	VAL
1	C	104	THR
1	C	109	LEU
1	C	126	LYS
1	C	128	ILE
1	C	137	ARG
1	C	149	LEU
1	C	154	THR
1	C	159	LEU
1	C	163	LEU
1	C	166	LYS
1	C	175	GLU
1	C	176	ARG
1	C	188	ARG
1	D	3	LEU
1	D	7	ARG
1	D	20	LEU
1	D	21	LEU
1	D	31	SER
1	D	34	SER
1	D	35	ILE
1	D	43	VAL
1	D	44	GLU
1	D	50	LEU
1	D	56	LEU
1	D	57	LEU
1	D	80	GLU
1	D	104	THR
1	D	114	ASP
1	D	118	GLU
1	D	121	ARG
1	D	127	LEU
1	D	128	ILE
1	D	139	LEU
1	D	141	VAL
1	D	159	LEU
1	D	163	LEU
1	D	164	ARG
1	D	165	LYS
1	D	171	ARG
1	D	175	GLU
1	D	177	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	186	VAL
1	E	2	ARG
1	E	7	ARG
1	E	10	LEU
1	E	20	LEU
1	E	25	ARG
1	E	33	LYS
1	E	48	GLN
1	E	50	LEU
1	E	57	LEU
1	E	58	GLU
1	E	74	CYS
1	E	79	GLN
1	E	88	LYS
1	E	99	ILE
1	E	104	THR
1	E	121	ARG
1	E	127	LEU
1	E	133	LYS
1	E	137	ARG
1	E	139	LEU
1	E	144	LYS
1	E	163	LEU
1	E	164	ARG
1	E	171	ARG
1	E	175	GLU
1	F	3	LEU
1	F	10	LEU
1	F	20	LEU
1	F	32	THR
1	F	44	GLU
1	F	56	LEU
1	F	57	LEU
1	F	58	GLU
1	F	65	GLU
1	F	68	GLU
1	F	69	ILE
1	F	74	CYS
1	F	75	ASN
1	F	80	GLU
1	F	88	LYS
1	F	109	LEU

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	118	GLU
1	F	120	ARG
1	F	121	ARG
1	F	128	ILE
1	F	141	VAL
1	F	149	LEU
1	F	160	VAL
1	F	163	LEU
1	F	175	GLU
1	F	177	THR
1	F	179	SER
1	F	186	VAL
1	F	190	ASN
1	G	2	ARG
1	G	6	CYS
1	G	7	ARG
1	G	20	LEU
1	G	25	ARG
1	G	34	SER
1	G	43	VAL
1	G	69	ILE
1	G	75	ASN
1	G	103	VAL
1	G	104	THR
1	G	109	LEU
1	G	126	LYS
1	G	128	ILE
1	G	149	LEU
1	G	154	THR
1	G	159	LEU
1	G	163	LEU
1	G	175	GLU
1	G	176	ARG
1	G	188	ARG
1	H	1	MET
1	H	7	ARG
1	H	20	LEU
1	H	21	LEU
1	H	31	SER
1	H	34	SER
1	H	35	ILE
1	H	43	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	44	GLU
1	H	50	LEU
1	H	52	LYS
1	H	56	LEU
1	H	57	LEU
1	H	80	GLU
1	H	104	THR
1	H	114	ASP
1	H	121	ARG
1	H	127	LEU
1	H	128	ILE
1	H	139	LEU
1	H	141	VAL
1	H	148	ARG
1	H	163	LEU
1	H	171	ARG
1	H	175	GLU
1	H	177	THR
1	H	186	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	B	79	GLN
1	B	110	ASN
1	D	79	GLN
1	E	39	HIS
1	F	110	ASN
1	H	79	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 [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	190/199 (95%)	-0.01	2 (1%) 80 80	70, 100, 132, 157	0
1	B	190/199 (95%)	-0.08	4 (2%) 63 61	61, 99, 141, 157	0
1	C	189/199 (94%)	-0.09	1 (0%) 91 90	68, 97, 134, 159	0
1	D	187/199 (93%)	-0.05	3 (1%) 72 69	75, 104, 137, 157	0
1	E	190/199 (95%)	-0.10	1 (0%) 91 90	69, 100, 131, 157	0
1	F	190/199 (95%)	-0.08	2 (1%) 80 80	57, 97, 138, 151	0
1	G	189/199 (94%)	-0.08	1 (0%) 91 90	70, 99, 139, 160	0
1	H	187/199 (93%)	0.09	5 (2%) 54 51	75, 102, 137, 157	0
All	All	1512/1592 (94%)	-0.05	19 (1%) 77 75	57, 100, 139, 160	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	97	PHE	4.5
1	B	69	ILE	4.4
1	H	152	PHE	3.5
1	H	85	ILE	3.4
1	H	112	PHE	3.2
1	A	108	PHE	3.2
1	D	97	PHE	2.9
1	A	103	VAL	2.8
1	H	108	PHE	2.8
1	B	99	ILE	2.4
1	E	159	LEU	2.4
1	B	183	ALA	2.3
1	G	127	LEU	2.3
1	B	68	GLU	2.2
1	D	50	LEU	2.2
1	F	99	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	109	LEU	2.1
1	F	69	ILE	2.0
1	D	124	LEU	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	MG	C	197	1/1	0.90	0.18	75,75,75,75	0
2	MG	F	197	1/1	0.91	0.12	95,95,95,95	0
2	MG	B	197	1/1	0.92	0.07	93,93,93,93	0
2	MG	D	197	1/1	0.94	0.07	90,90,90,90	0
2	MG	G	197	1/1	0.94	0.10	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.